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TECHNICAL REPORT ARBRL-TR-02302

TRANSPORT ALGORITHMS FOR PREMIXED, LAMINAR STEADY STATE FLAMES

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March 1981

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BALLISTIC RESEARCH LABORATORY
ABERDEEN PROVING GROUND, MARYLAND

UNCLASSIFIED

SECURITY CLASSIFICATION OF THIS PAGE (When Data Entered)

REPORT DOCUMENTATION PAGE

READ INSTRUCTIONS BEFORE COMPLETING FORM

1. REPORT NUMBER TECHNICAL REPORT ARBRL-TR-02302	2. GOVT ACCESSION NO.	3. RECIPIENT'S CATALOG NUMBER
4. TITLE (and Subtitle) TRANSPORT ALGORITHMS FOR PREMIXED, LAMINAR STEADY STATE FLAMES		5. TYPE OF REPORT & PERIOD COVERED BRL Technical Report 6. PERFORMING ORG. REPORT NUMBER
7. AUTHOR(s) T. P. Coffee J. M. Heimerl		8. CONTRACT OR GRANT NUMBER(s)
9. PERFORMING ORGANIZATION NAME AND ADDRESS U.S. Army Armament Resesearch & Development Command U.S. Army Ballistic Research Laboratory ATTN: DRDAR-BL Aberdeen Proving Ground, MD 21005		10. PROGRAM ELEMENT, PROJECT, TASK AREA & WORK UNIT NUMBERS 1L161102AH43
11. CONTROLLING OFFICE NAME AND ADDRESS U.S. Army Armament Research & Development Command U.S. Army Ballistic Research Laboratory ATTN: DRDAR-BLP Aberdeen Proving Ground, MD 21005		12. REPORT DATE MARCH 1981 13. NUMBER OF PAGES 161
14. MONITORING AGENCY NAME & ADDRESS(if different from Controlling Office)		15. SECURITY CLASS. (of this report) Unclassified 15a. DECLASSIFICATION/DOWNGRADING SCHEDULE

16. DISTRIBUTION STATEMENT (of this Report)

Approved for public release; distribution unlimited.

17. DISTRIBUTION STATEMENT (of the abstract entered in Block 20, if different from Report)

18. SUPPLEMENTARY NOTES

19. KEY WORDS (Continue on reverse side if necessary and identify by block number)

Laminar flames
Steady-state flames
Premixed flames
One-dimensional flames
Multicomponent transport algorithms
Diffusion velocity approximations
Thermal conductivity approximations
Thermal diffusion approximations

20. ABSTRACT (Continue on reverse side if necessary and identify by block number) (clt)

The effects of different methods of approximating multispecies transport phenomena in models of premixed, laminar, steady-state flames have been studied. Five approximation methods that span a wide range of computational complexity are developed. Identical data for individual species properties have been used for each method. Each approximation method is employed in the numerical solution of a set of five H_2-O_2-N_2 flames. For each flame the computed species and temperature profiles, as well as the computed flame speeds are found to be very

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20. ABSTRACT (Cont'd)

nearly independent of the approximation method used. This does not indicate that transport phenomena are unimportant, but rather that the selection of the input values for the individual species transport properies is more important than the selection of the method used to approximate the multispecies transport.

Based on these results we have developed a sixth approximation method that is computationally efficient and which provides results extremely close to the most sophisticated and precise method used.

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I. INTRODUCTION

To determine validated sets of elementary chemical reactions for use in predictive combustion models, we have chosen to simulate the one dimensional, premixed, laminar flame. This approach has the advantage that the predicted temperature and species profiles can in principal be compared with suitable burner experiments of the same flame. The corresponding equations are derived by Bird, Stewart and Lightfoot,[1] and by Williams,[2] and are given in Appendix A.

Such a simulation requires as input not only the kinetics information (of our immediate interest), but also thermodynamic and transport data. Fortunately the thermodynamics input is by and large well defined.[3,4] In addition, while some transport coefficients are only well defined through low temperature (< 1000 K) measurements,[5] the theory is sufficiently developed to allow reasonable estimates to be made at higher temperatures.[6] A theory has been developed for multicomponent

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[1] *R. B. Bird, W. S. Stewart and E. N. Lightfoot, Transport Phenomena, John Wiley and Sons, NY, (1960).*

[2] *F. A. Williams, Combustion Theory, Addison-Wesley, Reading, MA, (1965).*

[3] *D. R. Stull and H. Prophet, JANAF Thermochemical Tables, 2nd Edition, NSRDS-NBS-37, June 1971.*

[4] *S. Gordon and B. J. McBride, "Computer Program for Calculation of Complex Chemical Equilibrium Compositions, Rocket Performance, Incident and Reflected Shocks and Chapman-Jouguet Detonations", NASA-SP-273, (1971), (1976 program version).*

[5] *Y. S. Touloukian, P. E. Liley, and S. C. Saxena, Thermophysical Properties of Matter, Vol. 3, Thermal Conductivity (Nonmetallic Liquids and Gases), IFI/Plenum, NY-Washington, (1970).*

[6] *J. O. Hirshfelder, C. F. Curtiss and R. B. Bird, Molecular Theory of Gases and Liquids, 2nd printing, corrected, with notes, John Wiley and Sons, NY, (1964).*

mixtures,[6-10] but it is computationally cumbersome. To circumvent this, previous workers have generally employed some level of simplification.[11-21]

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[7] *C. S. Wang Chang, G. E. Uhlenbeck and J. deBoer, Studies in Statistical Mechanics, Vol. 2, John Wiley and Sons, NY, (1964).*

[8] *L. Monchick, K. S. Yun and E. A. Mason, "Formal Kinetic Theory of Transport Phenomena in Polyatomic Gas Mixtures", J. Chem. Phys., 39, 654-699 (1963).*

[9] *L. Monchick, A. N. G. Pereira and E. A. Mason, "Heat Conductivity in Polyatomic and Polar Gases and Gas Mixtures", J. Chem. Phys., 42, 3241-3256 (1965).*

[10] *L. Monchick, R. J. Munn and E. A. Mason, "Thermal Diffusion in Polyatomic Gases: A Generalized Stefan-Maxwell Diffusion Equation", J. Chem. Phys., 45, 3051-3058 (1966).*

[11] *G. Dixon-Lewis, et al., "Flame Structure and Flame Reaction Kinetics", Proc. R. Soc., London A 317, 235-263 (1970); A 330, 199-218 (1972); A 331, 571-584 (1973); and A 346, 261-278 (1975).*

[12] *G. Dixon-Lewis, "Kinetic Mechanism, Structure and Properties of Premixed Flames in Hydrogen-Oxygen-Nitrogen Mixtures", Phil. Trans. R. Soc., London, 292, 45-99 (1979).*

[13] *G. Tsatsaronis, "Prediction of Propagating Laminar Flames in Methane, Oxygen, Nitrogen Mixtures", Combust. and Flame, 33, 217-239 (1978).*

[14] *J. Warnatz, "Calculation of the Structure of Laminar Flat Flames 1; Flame Velocity of Freely Propagating Ozone Decomposition Flames", Ber. Bunsenges Phys. Chem., 82, 193-200 (1978).*

[15] *D. B. Spalding and P. L. Stephenson, "Laminar Flame Propagation in Hydrogen + Bromine Mixtures", Proc. R. Soc. London A, 324, 315-337 (1971).*

[16] *P. L. Stephenson and R. G. Taylor, "Laminar Flame Propagation in Hydrogen, Oxygen, Nitrogen Mixtures", Combust. and Flame 20, 231-244 (1973).*

[17] *L. D. Smoot, W. C. Hecker, and G. A. Williams, "Prediction of Propagating Methane-Air Flames", Combust. and Flame 26, 323-342 (1976).*

[18] *J. Warnatz, "Calculation of the Structure of Laminar Flat Flames II; Flame Velocity and Structure of Freely Propagating Hydrogen-Oxygen and Hydrogen-Air Flames", Ber. Bursenges Phys. Chem., 82, 643-649 (1978).*

[19] *D. B. Spalding, P. L. Stephenson, and R. G. Taylor, "A Calculation Procedure for the Prediction of Laminar Flame Speeds", Combust. and Flame 17, 55-64 (1971).*

[20] *L. Bledjian, "Computation of Time-Dependent Laminar Flame Structure", Combust. and Flame, 20, 5-17 (1973).*

[21] *E. Cramarossa and G. Dixon-Lewis, "Ozone Decomposition in Relation to the Problem of the Existance of Steady-State Flames", Combust. and Flame 16, 243-251 (1971).*

This paper addresses the question: which of the mathematical approximations to the multicomponent transport properties provides a desirable trade-off between precision and computational effort. Another way of phrasing this question is to ask what loss in precision of predicted flame speeds and profiles occurs as the mathematical approximations to the multicomponent, polyatomic transport expressions are made cruder.

We approach this problem by actually computing the flame properties for a given flame with a fixed set of input conditions. The transport algorithms are varied and the resulting flame speeds and profiles compared. The numerical method is discussed in references 22 and 23. We have selected the H_2-O_2-N_2 system as the candidate flame because it has a well characterized set of input parameters. (See Appendix B).

This paper is divided into the following sections. Section II outlines a sequence of five methods for approximating the transport coefficients. Section III shows the numerical results of these approximation methods relative to the most accurate method, and Section IV discusses their relative precision for a set of five flames. Based on these results, we outline in Section V an algorithm which provides a reasonable balance between computational effort and theoretical rigor and includes a crude approximation for the effects of thermal diffusion. There are several appendices that contain sufficient detail to reproduce our computations.

II. APPROXIMATION METHODS

In this section we outline five approximations to the multicomponent, polyatomic formalism, based on the theory of Wang Chang and Uhlenbeck.[6-10] We start with the most accurate and progressively consider cruder approximations. Method I is the three term Sonine approximation to the formalism. Dixon-Lewis (DL)[24] gives a discussion of this approximation, and we will generally follow his approach. Method II involves a level of approximation using smaller matrices. Methods III and IV use

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[22] *T. P. Coffee and J. M. Heimerl, "A Method for Computing the Flame Speed for a Laminar, Premixed, One Dimensional Flame", BRL Technical Report, ARBRL-TR-02212, Jan 80.*

[23] *T. P. Coffee, "A Computer Code for the Solution of the Equations Governing a Laminar, Premixed, One Dimensional Flame", BRL Memorandum Report, to be published.*

[24] *G. Dixon-Lewis, "Flame Structure and Flame Reaction Kinetics II. Transport Phenomena in Multicomponent Systems", Proc. Roy. Soc. A 307, 111-135 (1968).*

non-matrix techniques. Method V discusses the case of constant transport parameters. In each case we need to determine the diffusion velocities V_i, i = 1, 2, ... N, and the heat flux q.

A. Method I

Following (DL), we can write

$$q = \sum_{i=1}^{N} \rho Y_i V_i h_i - \lambda_o \frac{\partial T}{\partial x} - \sum_{i=1}^{N} \frac{RTD_i^T}{M_i Y_i} \frac{\partial X_i}{\partial x} \tag{1}$$

and

$$V_i = \frac{1}{X_i} \sum_{j=1}^{N} \frac{Y_j}{X_j} D_{ij} \frac{\partial X_j}{\partial x} - \frac{D_i^T}{\rho Y_i} \frac{\partial}{\partial x} (\ell n\ T), \tag{2a}$$

or

$$V_i = \mathcal{V}_i + \mathcal{W}_i, \tag{2b}$$

a notation we will later find convenient. The diffusion coefficients can be written in terms of the Sonine expansion coefficients,

$$D_{ij} = X_i \frac{16T}{25p} \frac{\sum_{k=1}^{N} M_k X_k}{M_j} c_{i00}^{1ji} \tag{3}$$

and

$$D_i^T = \frac{8}{5} \frac{M_i X_i}{R_a} a_{i00}^{1} . \tag{4}$$

Substituting equations (3) and (4) into equation (2) we find

$$V_i = \frac{16T}{25p} \sum_{j=1}^{N} (c_{i00}^{1ji} \frac{\partial X_j}{\partial x}) - \frac{8T}{5p} a_{i00}^{1} \frac{\partial}{\partial x} (\ell n\ T) . \tag{5}$$

Similarly, we can write

$$\lambda_o = \lambda_{o,tr} + \lambda_{o,int} = -4 \sum_{i=1}^{N} X_i\ a^1_{i10} - 4 \sum_{i=1}^{N} X_i a^1_{i01} \ . \qquad (6)$$

The diffusion velocities and the heat flux are now defined in terms of the a^1_{i00}, a^1_{i10}, a^1_{i01}, and c^{1ji}_{i00}. If we use three terms in the polynominal expansion, these are defined implicitly by the equations

$$(L)\ (a^1_{100} \ldots a^1_{N00}, a^1_{110} \ldots a^1_{N10}, a^1_{101} \ldots a^1_{N01})^T$$

$$= (0 \ldots 0, X_1 \ldots X_N, X_1 \ldots X_N)^T \qquad (7)$$

and

$$(L)\ (c^{1hk}_{100} \ldots c^{1hk}_{N00}, c^{1hk}_{110} \ldots c^{1hk}_{N10}, c^{1hk}_{101} \ldots c^{1hk}_{N01})^T$$

$$= (\delta_{1h} - \delta_{1k} \ldots \delta_{Nh} - \delta_{Nk}, 0 \ldots 0, 0 \ldots 0)\ h,k = 1 \ldots N. \qquad (8)$$

The elements of the 3N by 3N matrix (L) are given in Appendix C. The procedures we have used for computing these elements are discussed in Appendix D.

From equation (8), it appears that we must solve N^2 sets of equations to obtain the c^{1ji}_{i00}. In fact, it has been recommended[6,8,24] that only the a terms be computed using this level of approximation, and that the c terms be computed using a one term expansion (see Method II).

However, this is not necessary if we observe that we are only interested in the V_i's, and not directly in the c terms. We can convert the c-vector in equation (8) to a vector whose elements are in fact the V_i by multiplying each equation of (8) by $\frac{16T}{25p}\frac{\partial X_h}{\partial x}$ and then summing over h. After some algebra we find

$$(L)\ (V_1 \ldots V_N, \ldots\ldots)^T = \left(\frac{16T}{25p}\frac{\partial X_1}{\partial x} \ldots \frac{16T}{25p}\frac{\partial X_N}{\partial x}, 0 \ldots 0, 0 \ldots 0\right)^T. \qquad (9)$$

Equation (9) shows that we can solve directly for the required $\mathcal{V}_i$ and that the right hand side is not a function of either h or k.

In solving for the transport in our code, we decompose (L) as the product of an upper matrix multiplying a lower matrix. Equations (7) and (9) can then be solved efficiently by back substitution. It is computationally efficient to do this rather than generate another, smaller matrix for the $\mathcal{V}_i$ using a one term approximation and solving this new system. To solve these systems of algebraic equations we have used an assembly language algorithm[25] which has been found to execute on the BRL CDC 7600 about five times faster than the equivalent FORTRAN coding.

B. Method II

The above formalism is quite complicated to work with, and so further simplifications are almost invariably made.

For diffusion, we can simplify by taking only one term in the Sonine polynomial expansions. This results in

$$(L^{00,00})\ (c_{100}^{1hk}\ \ldots\ c_{N00}^{1hk})^T = (\delta_{1h}-\delta_{1k},\ \ldots\ \delta_{Nh}-\delta_{Nk})^T \quad h,k = 1\ \ldots\ N, \tag{10}$$

where the elements of $(L^{00,00})$ are defined in Appendix C. This can be rearranged[6] to give the Stefan-Maxwell equations, namely,

$$\frac{\partial X_i}{\partial x} = \sum_{j=1}^{N} \frac{X_i X_j}{\mathcal{D}_{ij}} (V_j - V_i),\ i=1\ \ldots\ N. \tag{11}$$

This set of equations is not independent, and the constraint

$$\sum_{i=1}^{N} Y_i V_i = 0 \tag{12}$$

must be used in place of one of the equations in (11). Then the diffusion velocities can be found by solving a set of N equations in N unknowns. This approach gives zero for the thermal diffusion velocity, $\mathcal{W}_i$.

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[25] *A. C. Hindmarsh, L. J. Sloan, K. W. Fong, and G. H. Rodrique, "DEC/SOL: Solution of Dense Systems of Linear Algebraic Equations", Lawrence Livermore Laboratory, UCID-30137, 1976.*

Thermal conductivity cannot be simplified this easily. However, ignoring internal energy, we can obtain the matrix form

$$L^{10,10}\,(a^{1}_{110}\,\ldots\,a^{1}_{N10})^{T} = (X_1,\,\ldots\,X_N)^{T}, \tag{13}$$

where $\lambda_o = \lambda_{o,tr} = -4 \sum_{i=1}^{N} X_i a^{1}_{i10}$.[26] This form will be valid for a mixture of monatomic gases.

To define the heat conductivity for a mixture of polyatomic gases, we adopt Hirshfelder's* Eucken-type relation,[27,5]

$$\lambda^{poly}_{mix} = \lambda^{mon}_{mix} + \sum_{i=1}^{N} \frac{\lambda_i - \lambda_i^{mon}}{1 + \sum\limits_{j\neq i} \dfrac{\mathcal{D}_{ii}}{\mathcal{D}_{ij}} \dfrac{X_j}{X_i}} \;. \tag{14}$$

The quantity λ_o in method I is not exactly identical to the usual thermal conductivity λ^{poly}_{mix}, but can be interpreted as the thermal conductivity of a mixture in which the diffusion forces vanish.

If the thermal diffusion coefficients are zero, as they are at this level of approximation, then $\lambda_o = \lambda^{poly}_{mix}$.

C. Method III

By making additional assumptions, the Stefan-Maxwell equations (11) can be further simplified. A common assumption is that all but the i^{th} species move with the same velocity V. Then we find that

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The detailed analysis of Monchick, et al.,[9] shows that the $\mathcal{D}_{ij}$ should be $\mathcal{D}_{i,int,j}$. From a practical point of view we have taken $\mathcal{D}_{i,int,j} = \mathcal{D}_{ij}$.

[26] *C. Muckenfuss and C. F. Curtiss, "Thermal Conductivity of Multicomponent Gas Mixtures", J. Chem. Phys. 29, 1273-1277 (1958).*

[27] *J. O. Hirshfelder, "Heat Conductivity in Polyatomic, Electronically Excited, or Chemical Reacting Mixtures. III", Sixth International Combustion Symposium, Reinhold Publishing Corporation, NY, 351-366 (1957).*

$$\frac{\partial X_i}{\partial x} = X_i \; (V - V_i) \sum_{j \neq i} \frac{X_j}{\mathcal{D}_{ij}} \; . \qquad (15)$$

Employing (12) we find

$$V = - \frac{Y_i V_i}{1 - Y_i} \qquad (16)$$

which when substituted into (15) yields the formula recommended by Hirshfelder and Curtiss[28]

$$V_i = - \frac{(1 - Y_i)}{X_i \sum_{j \neq i} \frac{X_j}{\mathcal{D}_{ij}}} \frac{\partial X_i}{\partial x} . \qquad (17)$$

Unfortunately, the expression in (17) does not in general satisfy equation (12). One technique to satisfy this constraint is due to Boris and Oran.[29] They note that if a set of diffusion velocities V_i satisfy the Stefan-Maxwell equations (11), then so does the set $(V_i + V_c)$, where V_c is some constant. The value of V_c is chosen such that the constraint (12) is satisfied.*

The heat conductivity formula employed at this level of approximation is taken from Mason and Saxena's[30,5] simplification of (14), specifically

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[28] *J. O. Hirshelder and C. F. Curtiss, "Theory of Propagation of Flames Part I: General Equations", Third International Combustion Symposium, Williams and Wilkins Co., Baltimore, 121-127 (1949).*

[29] *E. S. Oran and J. P. Boris, "Detailed Modeling of Combustion Systems", to appear in Progress in Energy and Combustion Science.*

* *Boris and Oran also discuss higher order approximations to the Stefan-Maxwell equations that will not be discussed here.*

[30] *E. A. Mason and S. C. Saxena, "Approximate Formula for the Thermal Conductivity of Gas Mixtures", Phys. Fluids, 1, 361-369 (1958).*

$$\lambda_o = \sum_{i=1}^{N} \frac{\lambda_i}{1 + \sum_{j\neq i} \phi_{ij} \; (X_j/X_i)} \tag{18}$$

where

$$\phi_{ij} = \frac{1.065}{8^{\frac{1}{2}}} \left(1 + \frac{M_i}{M_j}\right)^{-\frac{1}{2}} \left[1 + \left(\frac{\eta_i M_j}{\eta_j M_i}\right)^{\frac{1}{2}} \left(\frac{M_i}{M_j}\right)^{\frac{1}{4}}\right]^2 . \tag{19}$$

D. Method IV

Equation (17) or some analogous form has often been used to compute diffusion. However, the usual procedure has been to use (17) only to compute $V_1, \ldots, V_{N-1}$. Then V_N is computed from (12). This is less accurate than the Boris and Oran procedure, expecially for V_N.

Also, an empirical formula for the thermal conductivity,

$$\lambda_o = 0.5 \left[\sum_{i=1}^{N} X_i \lambda_i + \left\{ \sum_{i=1}^{N} X_i/\lambda_i \right\}^{-1} \right] , \tag{20}$$

is often used.[31,5]

Method IV is comprised of these common approximations.

E. Method V

In the case of a binary mixture the Stefan-Maxwell equations (11) reduce to Fick's law. Specifically we have,

$$Y_1 V_1 = -\mathcal{D}_{12} \frac{\partial Y_1}{\partial x} . \tag{21}$$

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[31] *J. H. Burgoyne and F. Weinber, "A Method of Analysis of a Plane Combustion Wave", Fourth Symposium on Combustion, Williams and Wilkins Co., Baltimore, 294-302 (1953).*

A generalization of (21) can be made,[1] and yields

$$Y_i V_i = -D_{im} \frac{\partial Y_i}{\partial x} , \tag{22}$$

where

$$D_{im} = \frac{1 - X_i}{\sum_{j \neq i} \frac{X_j}{\mathcal{D}_{ij}}} . \tag{23}$$

In the Lennard-Jones formalism $\mathcal{D}_{ij} \propto T^{1.5}/\Omega^{(1,1)*}$, where $\Omega^{(1,1)*}$ is approximately proportional to $T^{-0.17}$.[32] Since $\rho \propto T^{-1}$ it is not unreasonable to assume that $\rho^2 \mathcal{D}_{ij}$ is approximately independent of temperature. Generalizing, it is often assumed that $(\rho^2 D_{im})$ is constant. Likewise for a monatomic gas $\lambda \propto T^{0.5}/\Omega^{(2,2)*}$, where $\Omega^{(2,2)*} \propto T^{-0.16}$,[32] and it is not unreasonable to assume that $(\rho\lambda)$ is approximately independent of temperature. We now outline a procedure that permits an *a priori* selection of these quantities.

For a given flame we know T_u and Y_{iu}, the temperature and the mass fractions of the unburned mixture. We also have a chemical kinetics scheme and a method of computing the specific heats c_{pi} and specific enthalpies h_i. Since enthalpy is conserved, i.e.,

$$\left(\sum_{i=1}^{N} Y_i h_i\right)_B = \left(\sum_{i=1}^{N} Y_i h_i\right)_u , \tag{24}$$

we can compute the adiabatic flame temperature T_B. The numerical procedure is to guess a trial burned temperature T_t and, using an ODE package, find the corresponding equilibrium mass fractions Y_{it}. We then compute the enthalpy of the burned mixture and compare with the unburned mixture enthalpy. T_t is iteratively adjusted until the burned and unburned mixture enthalpies agree to within a pre-determined error tolerance. We then accept these values of T_t and Y_{it} as T_B and Y_{iB}.

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[32] *A. A. Westenberg, "Present Status of Information on Transport Properties Applicable to Combustion Research", Combustion and Flame, 1, 346-358 (1957).*

At this level of approximation we would like to use an appropriate constant (or "global") c_p. So we will assume that $c_{pi} = c_p$ = constant, $i = 1 \ldots N$. Then the relation $h_i = h_i^\circ + \int_{T_o}^{T} c_{pi}\, dT$ becomes $h_i = h_i^\circ + c_p (T - T_o)$ and the mixture enthalpy is given by

$$\sum_{i=1}^{N} Y_i h_i = \sum_{i=1}^{N} Y_i h_i^\circ + c_p (T - T_o) \quad . \tag{25}$$

Substituting (25) into (24) we find

$$c_p = \frac{\sum_{i=1}^{N} h_i^\circ (Y_{iu} - Y_{iB})}{T_B - T_u} \quad . \tag{26}$$

As a heuristic rule, we select $T = 0.5\ (T_B + T_u)$ and $Y_i = 0.5\ (Y_{iB} + Y_{iu})$ and then evaluate D_{im} and $\rho\lambda$ by using equations (23) and (20), respectively. Then $\rho^2 D_{im}$, $i = 1,2,\ldots N-1$, and $\rho\lambda$ are evaluated. The diffusion velocity V_N is found from equation (12).

Others[19-21] have employed the concept of constant $\rho^2 D_{im}$, $\rho\lambda$ and c_p, but the method of evaluation varies from author to author.

III. NUMERICAL RESULTS

Table 1 shows a summary of the five methods of computing the transport properties used in this paper. Five H_2-O_2-N_2 flames were selected and their initial conditions listed in Table 2. The total pressure is fixed at one atmosphere for all flames. The computed flame speed for each flame as a function of transport method is tabulated in Table 3. (The flame speeds for flame A are not corrected to 291 K, as has been done.[11] If this were done, the value AI for example would be 12.2 cm/s instead of 14.1 cm/s.) The values of the flame speeds span a large range and for a given flame are essentially independent of the transport method. The largest difference between Method I, the most complete formulation of the transport, and any other method is 16%. (Compare Methods I and III, flame D). Note that even Method V gives results that are quite close to the much more complex Method I.

TABLE 1. SUMMARY OF TRANSPORT METHODS

Method	Remarks
I	3 terms of Sonine polynomial expansion (3 N by 3 N matrix); only method that has non-zero thermal diffusion.
II	For diffusion, 1 term of Sonine polynomial expansion (N by N matrix), Eq. (11) and (12). For thermal conductivity, Hirshfelder-Eucken method (N by N matrix), Eq. (13) and (14).
III	Diffusion velocities computed from simplified Stefan-Maxwell relation, Eq. (17). Each is adjusted by a common factor, V_c, so as to satisfy $\sum_{i=1}^{N} Y_i V_i = 0$. Thermal conductivity from Mason and Saxena, Eq. (18) and (19).
IV	Diffusion velocities computed from the simplified Stefan-Maxwell relation, Eq. (17), for N-1 species. V_N is computed from Eq. (12). Empirical thermal conductivity formula, Eq. (20).
V	$\rho^2 D_{im}$ = constant; $\rho\lambda$ = constant; c_p = constant; constants are determined *a priori*.

TABLE 2. INITIAL TEMPERATURE AND MOLE FRACTIONS FOR THE FIVE FLAMES STUDIED

Flame	X_{H2}	X_{O2}	X_{N2}	T_u
A	.1883	.0460	.7657	336
B	.2000	.1680	.6320	298
C	.5000	.1050	.3950	298
D	.9000	.1000	0	298
E	.6000	.4000	0	298

TABLE 3. FLAME SPEEDS CALCULATED USING THE FIVE TRANSPORT MODELS

Flame	I	II	III	IV	V
A	14.1	14.6	14.9	14.9	16.0
B	98	101	102	103	96
C	292	300	310	308	291
D	378	379	438	402	348
E	892	922	971	969	847

Reproduction of flame speeds is a necessary but not sufficient condition to judge the relative effectiveness of the transport methods. We must also examine the species and temperature profiles of these flames. As examples we consider two sets of profiles that exhibit differences among the five methods that are as large as any observed. Figures 1 and 2 show the OH profiles for flame D. Figures 3 and 4 show the H_2 profiles for flame C. As can be seen these profiles are very similar. Almost all the other species profiles and all temperature profiles show a greater degree of similarity among the five profiles than the examples given.

In general, our results agree with those reported by Warnatz.[18] The exception is flame A, for which Warnatz reported a flame speed of 10.4 cm/sec, referenced to 291K. Our computed flame speed is about twenty percent higher. Based on our results, we infer that Warnatz's use of a transport method slightly different from any of those reported here should not make that large a difference. We do not know the cause of the discrepancy.

As a check of our code, we computed the flame speed for flame A, using the kinetics and transport parameters of Dixon-Lewis[12] and Method I. The resulting flame speed was 9.2 cm/sec, referenced to 291K. This agrees with the computed result reported by Dixon-Lewis and we conclude that our code is functioning properly.

We are comparing the model results produced as we vary the transport algorithm and <u>not</u> comparing the model result with experiment. Thus, the fact that the use of Warnatz' parameters produces a slightly inaccurate flame speed for flame A is of no concern.

IV. DISCUSSION

The numerical results shown in Table 3 demonstrate that reliable results can be obtained for the H_2-O_2-N_2 system even for the case of our *a priori* determined constant transport method. Note that we cannot infer that transport is unimportant! The computed profiles and flame speeds can be sensitive to the choice of transport parameters selected. For the relative tests of the transport methods here, we have employed the same set of species viscosities, thermal conductivities and binary diffusion coefficients in all cases. We have demonstrated that the method used to generate the multicomponent, polyatomic transport coefficients is not critical for the H_2-O_2-N_2 flame. And since this flame is reasonably complex we infer that this result has a high probability of being valid for other flames.

Indeed, we conclude that gross errors detected in comparing the results of different models are more likely to be traceable to differences in input data rather than to the method of approximating multicomponent polyatomic transport properties.

We cannot completely explain the surprising agreement among the

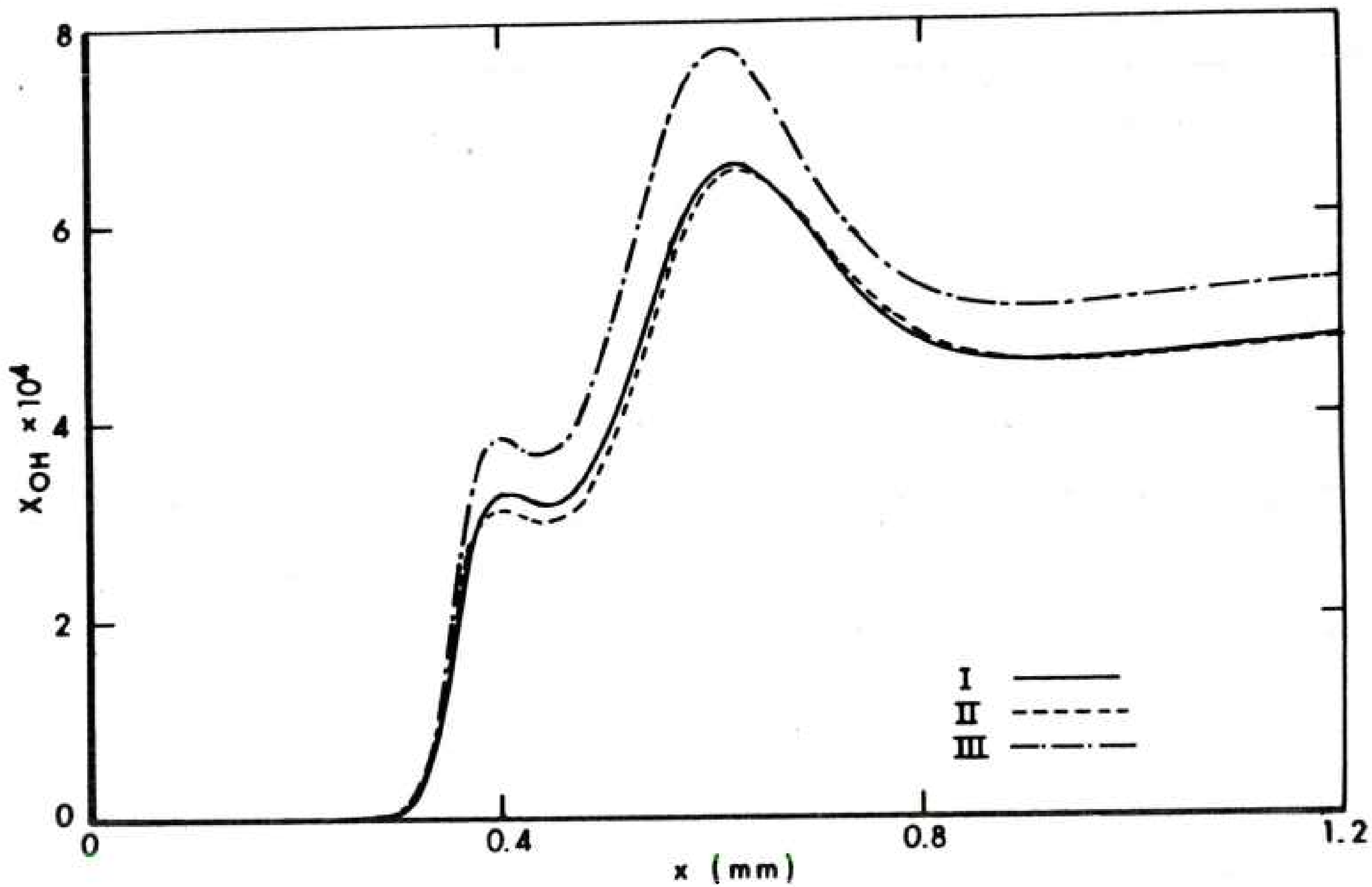

Figure 1. The OH Profile for Flame D.

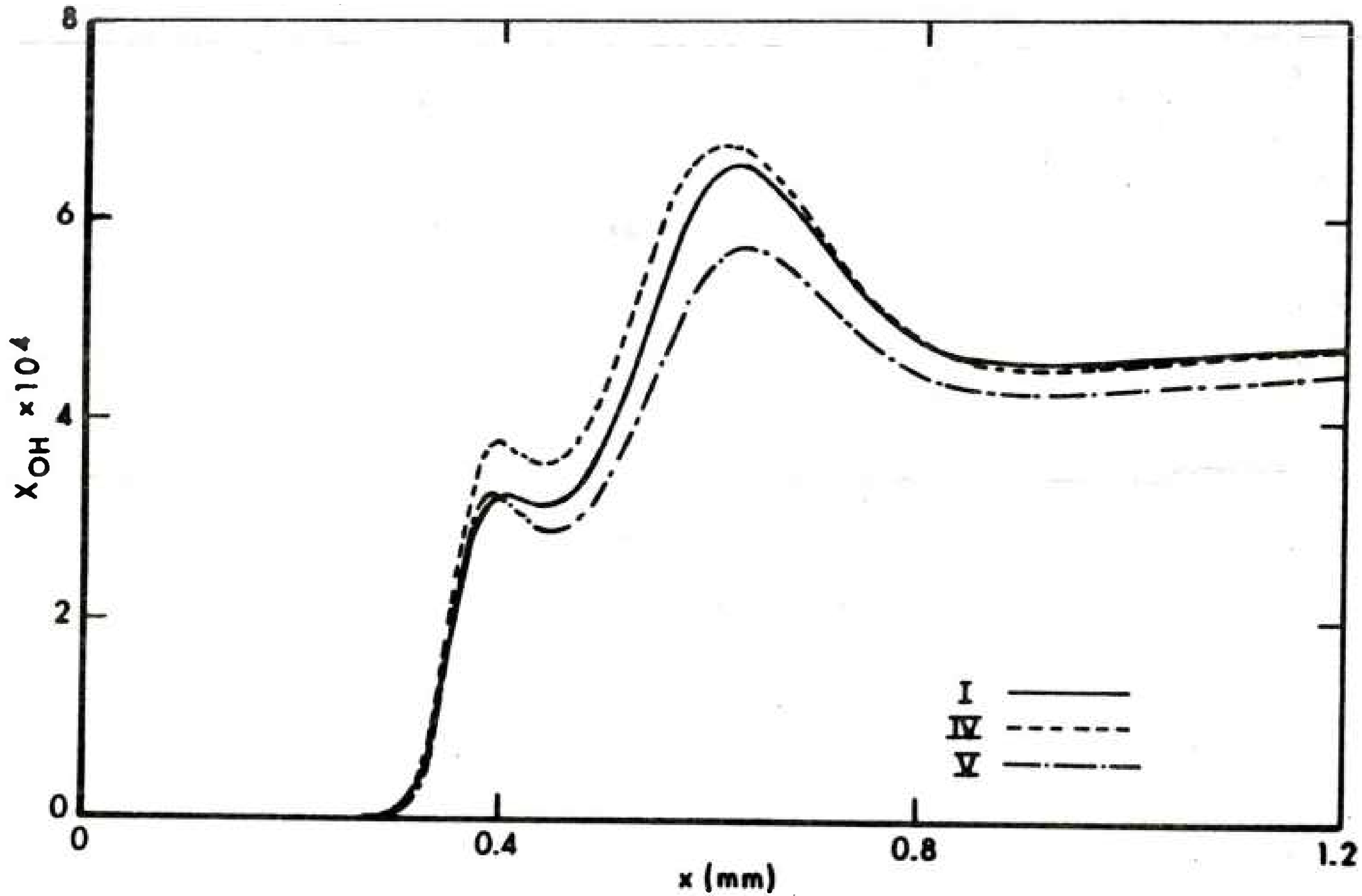

Figure 2. The OH Profile for Flame D.

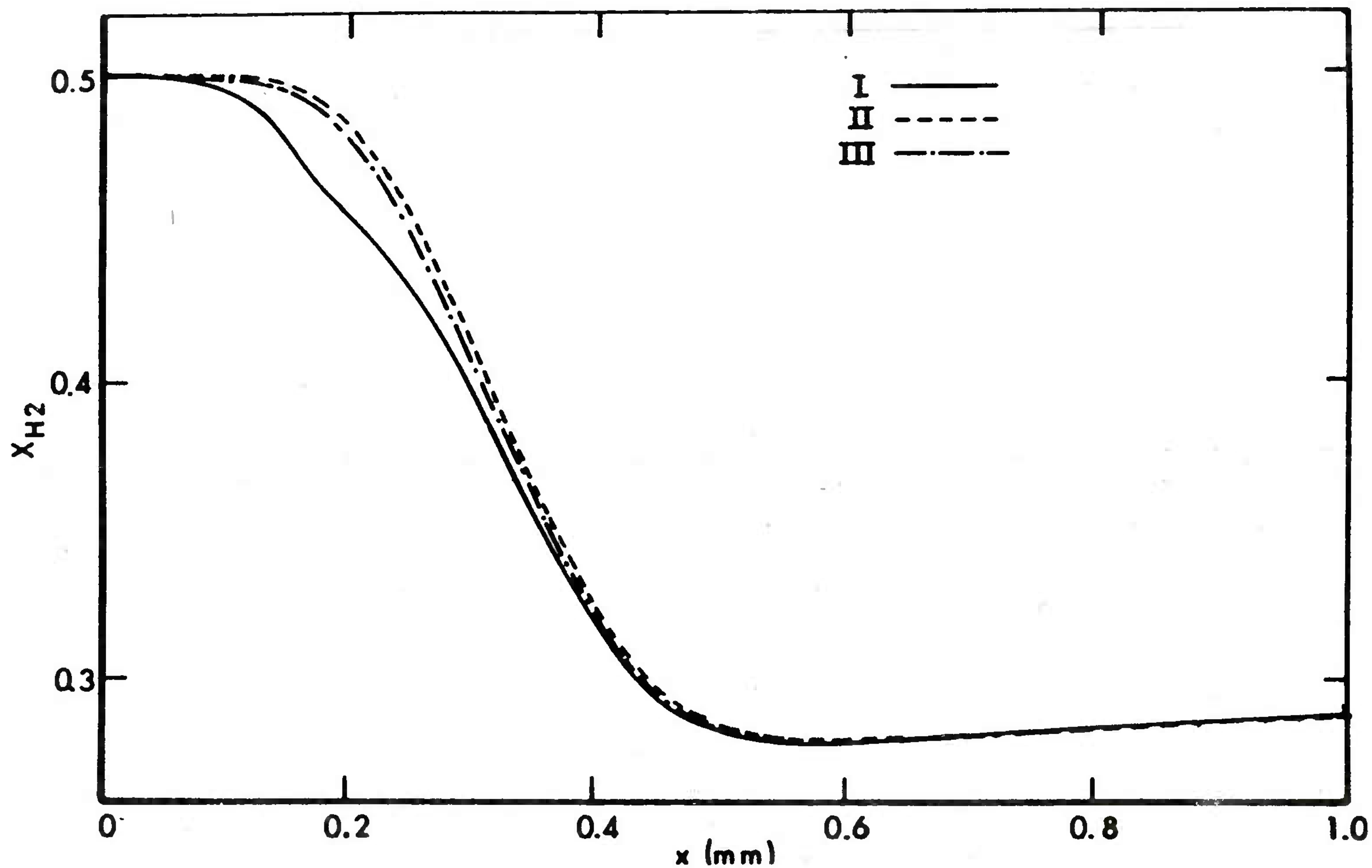

Figure 3. The H_2 Profile for Flame C.

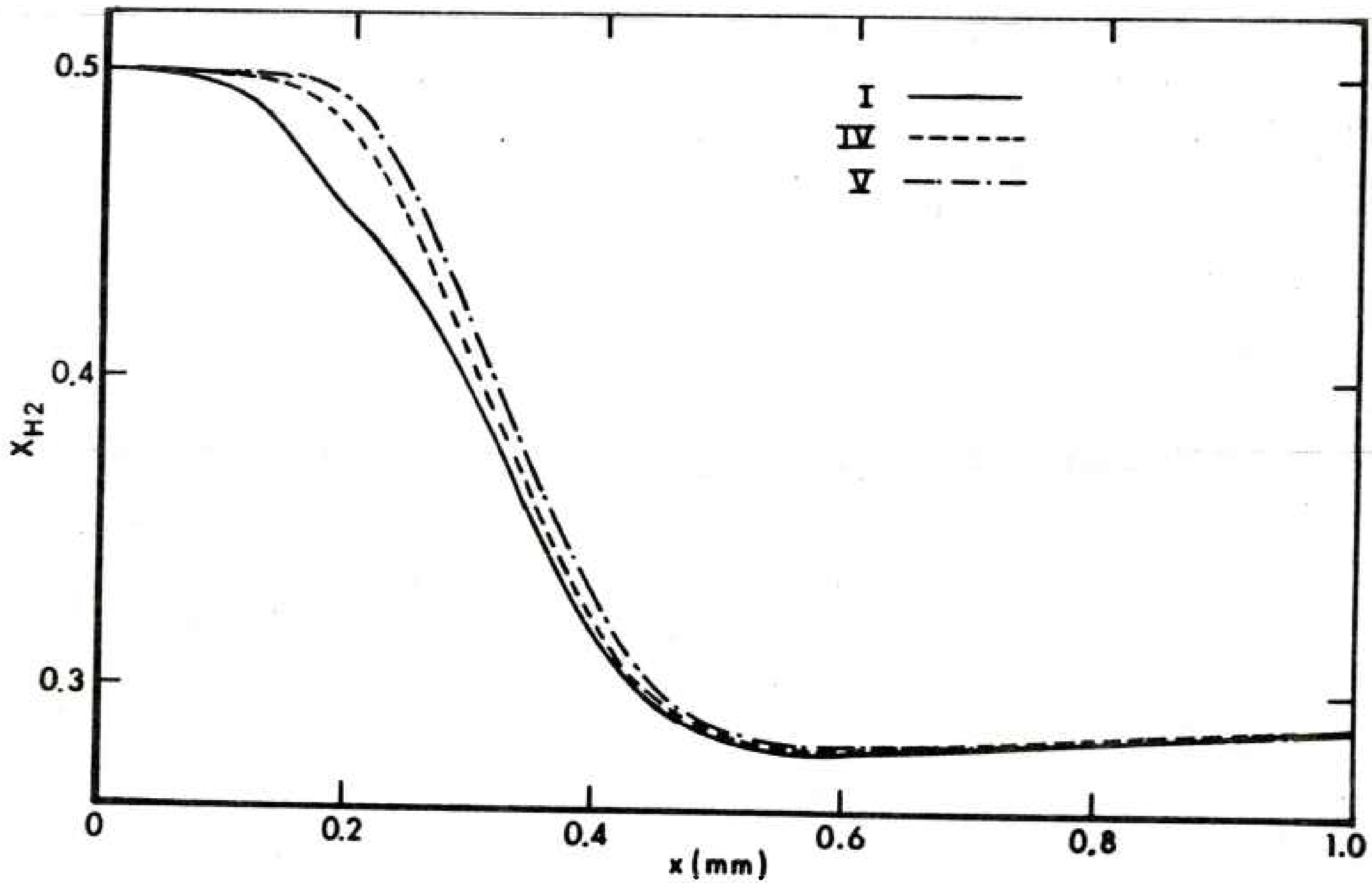

Figure 4. The H_2 Profile for Flame C

various methods. In this section we will show that our results are consistent with the few previous studies of transport algorithms. We will also discuss some additional numerical results that give some indication of the processes involved.

Warnatz[14] essentially compared Methods II and III for an ozone flame and found the differences negligible. However, it was not clear that his observations could be generalized to more complex flames.

In another paper[18] Warnatz included thermal diffusion in a simulation of an H_2-O_2-N_2 flame. He used essentially Method IV together with a simple binary formula for thermal diffusion valid only for heavy isotopes.[6] He found that the effect of thermal diffusion so defined was to lower the flame speed in a rich flame by about 5%. Species and temperature profiles were only slightly changed. He did not discuss the accuracy of this approximation for a mixture.

As noted earlier, Dixon-Lewis[24] considered the effect of thermal diffusion. However, he assumed a particular mass flow and simplified chemistry. He found that the thermal diffusion flux of H_2 was quite large and inferred that effects due to thermal diffusion would be important when considering hydrogen atom diffusion in flame systems. This inference is contrary to our findings. Our results also show that, for H and H_2, the thermal diffusion velocity W_i can be quite large compared to the species diffusion velocity V_i. However, we find that these differences cause only small changes in both the flame speeds and the profiles. This finding supports that of Dixon-Lewis[12] who in a recent paper reported that the inclusion of thermal diffusion for near stoichiometric H_2-air flames lowers the burning velocity by 5 to 6%.

In an attempt to gain additional insight, we have written an auxilary code to directly compare the transport properties. The input required for this code are the values of the temperature, the species concentrations, and the temperature and species gradients. Then the thermal conductivity λ_o and the diffusion velocities V_i are computed using the subroutines written for Methods I through IV, and comparisons among the values for λ_o and V_i are made. By doing this we avoid the complicated interplay between transport and chemistry that occurs in flames.

The auxiliary code was executed using several hundred sets of input values that were typical of those observed in the flames reported above. These input values were divided into four groups for analysis. Group 1 consisted of small species and temperature gradients, Group 2 of large species and temperature gradients, Group 3 of large species gradients and a zero temperature gradient, and Group 4 of small species gradients and large temperature gradients. By a large gradient we mean a value typical of a flame front.

The values of thermal conductivity computed with the auxiliary code showed little variation, regardless of the input group or approximation method used. Specifically, the differences between Methods I and II, I and III, and I and IV averaged 2, 3 and 5%, respectively. In general, the thermal conductivities of the individual species are not this well known either theoretically or experimentally. So despite the widely different levels of complexity, the four methods produced equivalent values for λ_o.

The results of the comparisons for diffusion velocities are more difficult to summarize. Differences varied from less than 1% up to several hundred percent, depending on the particular input values and the particular species considered. Differences of 30 to 40% were common and in general were larger for the major species than for the minor species.

We could not establish why there was a high degree of similarity in the flame speeds and profiles even though these were large differences in the V_i in the auxiliary code. We speculate that part of the reason for this is due to the constraint $\sum_{i=1}^{N} Y_i V_i = 0$, which is satisfied by all of our methods. Another constraint on the diffusion velocities in the flame code is the fixed chemistry employed. How the non-linear feedback between the chemistry and the transport affects the similarity in the flame speeds and profiles is unknown.

Nevertheless, some interesting conclusions can be drawn from these comparisons. For instance, it is often assumed that thermal diffusion is negligible. This assumption corresponds to that made in Group 3. (If the temperature gradient is zero, the thermal diffusion velocities W_i will also be zero).

For this group, we find that the values of the diffusion velocities computed by Methods I and II agree to about 1%. In contrast, the values of the diffusion velocities computed by Methods III and IV differ from those computed by Method I by much more (typical differences are around 40%). This comparison implies that Method II (i.e., the Stefan-Maxwell equations) is much more accurate in determining the values for the diffusion velocities than the non-matrix methods. Note that this conclusion is valid only for the case of zero temperature gradient.

For the other three groups of input to our auxiliary code, we find that the diffusion velocities computed by Method III are usually in better agreement with those computed by Method I than those computed by Method II! This situation can occur because in Method III the errors in ignoring thermal diffusion and in approximating the molecular diffusion velocities are generally of opposite sign. We conclude that it is a waste of effort to use a matrix method (such as the Stefan-Maxwell equations) to compute diffusion velocities unless thermal diffusion is also considered.

Method III is generally more accurate than Method IV. Method IV can be extremely inaccurate in computing the diffusion velocity for the

Nth species. In the cases considered we have found that the values computed by Method IV for N_2 differ, on the average, more than 100% from the values found by Method I. This is due to the procedure used to obtain the diffusion velocity for the Nth species. This procedure tends to associate cumulative errors caused by neglect of the constraint, Eq. (12), with the Nth species, here N_2. We have found that Method III (the Boris and Oran procedure) is at least as accurate and in some cases substantially more accurate than the traditional Method IV for computing the V_i. Furthermore the Boris and Oran procedure involves very little additional computational effort.

V. A NEW TRANSPORT METHOD

For flames more complicated than H_2-O_2-N_2 we require a transport algorithm that is computationally efficient and relatively precise. The most exact procedure considered, Method I, can become prohibitively expensive for a large number of species. Method V is computationally efficient, but we feel caution is necessary in using such a simplified model. There does not seem to be a great deal to choose from among Methods II, III, and IV and so we have assembled a new method, Method VI.

As with Methods II-V we require expressions for λ_o and for the $V_i(= \mathcal{V}_i + \mathcal{W}_i)$. For the thermal conductivity we use the simplest formula (20), since the exact choice does not appear to be important. For the molecular diffusion velocities $\mathcal{V}_i$ we use the expression in equation (17).

For problems with light species and steep temperature gradients, the neglect of thermal diffusion is often as important as the differences between the computational methods. So below we generate a technique that approximates the thermal diffusion contribution to the diffusion velocity, $\mathcal{W}_i$. We shall first derive an expression for $\mathcal{W}_i$ of a binary mixture and then generalize the results.

For a binary mixture equation (2a) can be written

$$V_1 = - \frac{(1-Y_1)}{X_1 X_2} \mathcal{D}_{12} \frac{\partial X_1}{\partial x} - \frac{D_1^T}{\rho Y_1} \frac{\partial \ln T}{\partial x} \tag{27}$$

from which we identify

$$\mathcal{W}_1 = - \frac{D_1^T}{\rho Y_1} \frac{\partial \ln T}{\partial x} . \tag{28}$$

Since, from Eq. (17),

$$\mathcal{V}_1 = -\frac{(1-Y_1)}{X_1 X_2} \mathcal{D}_{12} \frac{\partial X_1}{\partial x} \tag{29}$$

and since the thermal diffusion ratio is defined by reference 6

$$k_{12} = \frac{X_1 X_2}{\rho Y_1 Y_2} \frac{D_1^T}{\mathcal{D}_{12}} \quad , \tag{30}$$

we can write, after some algebra,

$$\mathcal{W}_1 = k_{12} \mathcal{V}_1 \frac{\partial}{\partial x} (\ell n T) / \frac{\partial X_1}{\partial x} \quad . \tag{31}$$

Theoretical expressions for k_{12} have been derived and even in the first approximation the expressions are quite complicated.[6] For the special case of heavy isotopes, however, the first approximation simplifies to[6]

$$k_{12} = \frac{15(2A^* + 5)(6C^* - 5)}{2A^*(16A^* - 12B^* + 55)} \frac{(M_1 - M_2)}{(M_1 + M_2)} X_1 X_2 \quad . \tag{32}$$

Fortunately Eq. (32) reproduces H_2-N_2 thermal diffusion ratios to within 30%, and so we use it as a simple but reasonable approximation for k_{12}. Equation (31) can now be evaluated (in the code).

Generalizing Eq. (31) we define

$$\mathcal{W}_i \equiv k_{im} \mathcal{V}_i \frac{\partial}{\partial x} (\ell n T) / \frac{\partial X_i}{\partial x} \quad . \tag{33}$$

If an expression for k_{im} can be obtained, then $\mathcal{W}_i$ of Eq. (33) can be evaluated. Chapman and Cowling[33] have derived an approximation for k_{im},

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[33] *S. Chapman and T.G. Cowling, The Mathematical Theory of Non-Uniform Gases, Third Edition, Cambridge University Press (1970).*

specifically

$$k_{im} = \sum_{\substack{j=1 \\ i \neq j}}^{N} k_{ij} \tag{34}$$

where k_{ij} is given by an expression analogous to Eq. (32).

From Eq. (32) we can see that the influence of W_i will be the greater the larger the mass differences. Normally the thermal diffusion ratio does not exceed 0.1 and for the H_2-O_2-N_2 system, we have computed W_i only for the species H and H_2. The resulting diffusion velocities $V_i = V_i + W_i$ do not satisfy the constraint $\sum_{i=1}^{N} Y_i V_i = 0$. We use the Boris and Oran procedure discussed in Section II to obtain this condition.

Computationally, the quantity 15(2A* + 5)/(2A*(16A* - 12B* + 55)) can be fitted very accurately by a function of the form: a exp (c/T*). The quantity (6C* - 5) varies over the range zero to one and could not be fitted accurately by a simple expression. The fit for C* given in Appendix D is used instead.

This new method for approximating multispecies transport has been exercised in our test flames. Table 4 compares the flame speeds for Methods I and VI. The results are so close that we infer that some of the errors made in the approximations involved in Method VI are cancelling.

Figure 5 compares the OH profiles for flame D and figure 6 compares the H_2 profiles for flame C. In general, for the minor species, the accuracy of Method VI is comparable to Methods II or III. However, in almost every profile involving a major species, the accuracy was improved.

VI. ADDENDUM

A few additional comparisons have recently been made. In the spirit of approximation exemplified in the discussion of Method V, the further assumption is sometimes made that all the Lewis numbers ($Le_i = \lambda/c_p \rho D_{im}$) are equal to unity. Given values for $\rho\lambda$ and c_p, this assumption defines the diffusion coefficients and removes the requirement of supplying independent information for them. We tested how well this additional level of simplification fared by applying it in the code using flame C. The computed flame speed was about 40% lower than for Method I. While the major species profiles were still reasonably close to those of Method I, they were noticeably less accurate than Method V. The minor species profiles showed large differences: the peak concentrations of O, HO_2, and H_2O_2 were lower than those of Method I by about a factor of two.

In an effort to substantiate our earlier inference concerning the transfer of these results to other (hydrocarbon) flames we performed some checks on the stoichiometric methane-air flame. For this flame we used the input parameters listed by Tsatsaronis,[13] the kinetics scheme was used as listed, and we made no attempt to critically evaluate it. The flame speeds computed for Methods I, V, and VI are in the ratio 1.00 to 0.88 to 0.94, respectively. The profiles for Method VI are more accurate than those produced by Method V. These results follow the same trend as in the H_2-O_2-N_2 flames reported above.

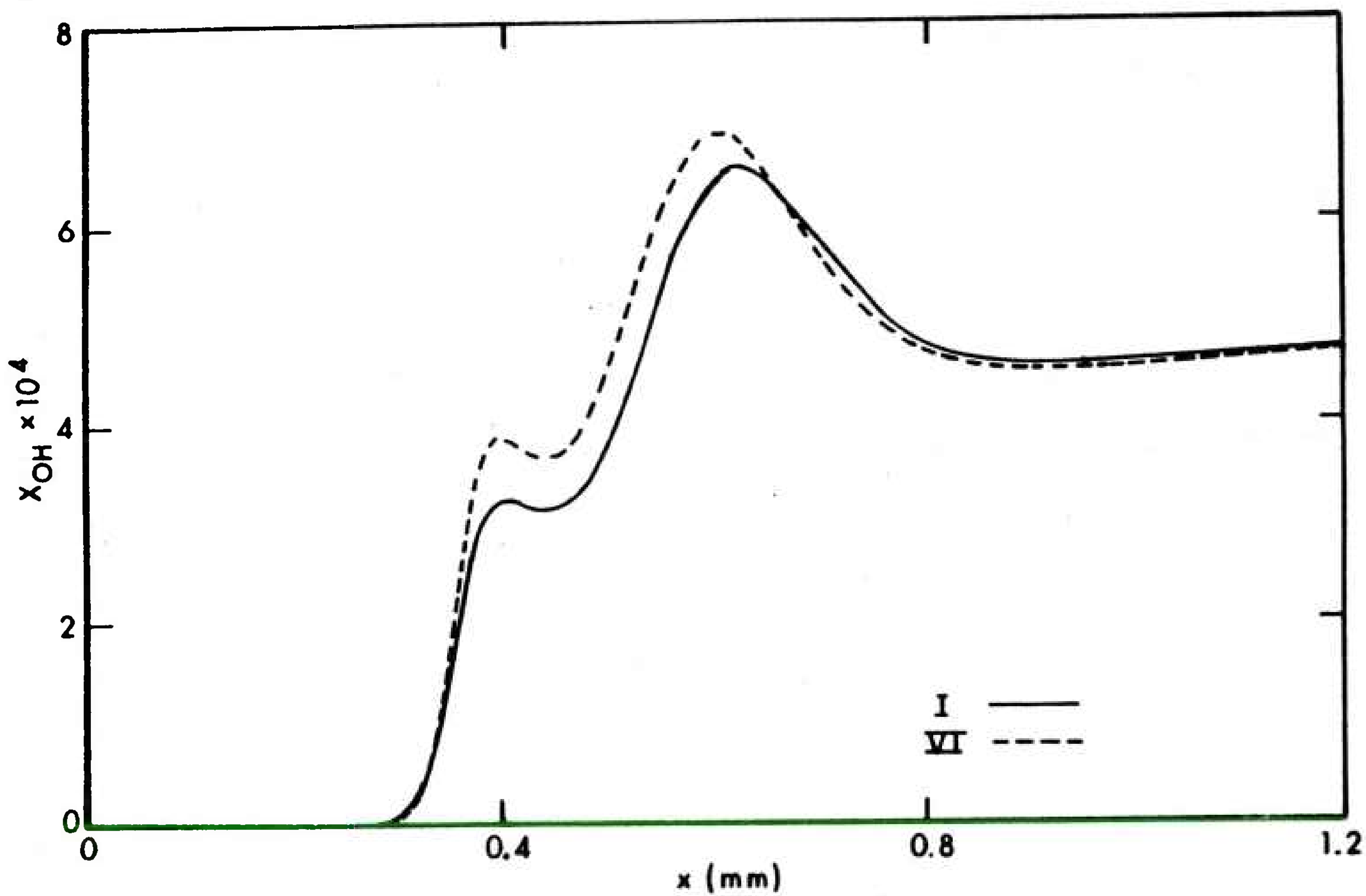

Figure 5. The OH Profile for Flame D.

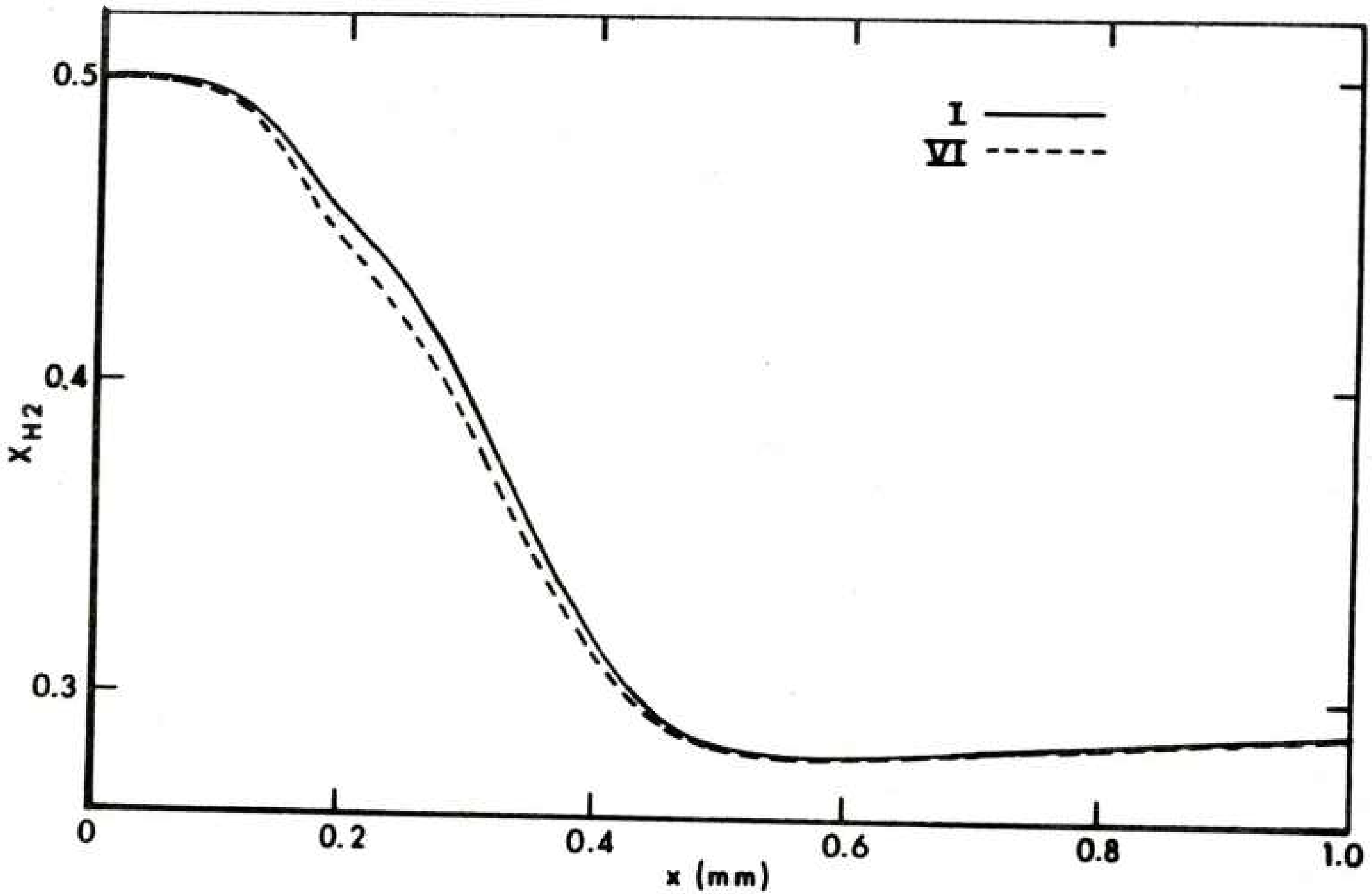

Figure 6. The H_2 Profile for Flame C.

TABLE 4. FLAME SPEEDS CALCULATED USING TWO TRANSPORT MODELS

Flame	I	VI
A	14.1	14.0
B	98	97
C	292	292
D	378	402
E	892	894

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APPENDIX A. THE FLAME EQUATIONS

We are interested in the equations that describe a one-dimensional, laminar, premixed flame that propagates in an unbounded ideal gas. The effects of radiation, viscosity, and body forces are ignored. Since the burning velocity is small compared with the local speed of sound, the pressure is taken to be constant. The resulting equations (see for example reference 2 of text) are:

Overall Continity:

$$\frac{\partial \rho}{\partial t} + \frac{\partial (\rho u)}{\partial x} = 0 \quad . \tag{A-1}$$

Continuity of Species:

$$\rho \frac{\partial Y_i}{\partial t} + \rho u \frac{\partial Y_i}{\partial x} = - \frac{\partial}{\partial x} (\rho Y_i V_i) + R_i M_i , \; i = 1, \ldots N \quad . \tag{A-2}$$

and Conservation of Energy:

$$\rho c_\rho \frac{\partial T}{\partial t} + \rho u c_\rho \frac{\partial T}{\partial x} = - \frac{\partial q}{\partial x} + \sum_{i=1}^{N} h_i \left[\frac{\partial (\rho Y_i V_i)}{\partial x} - R_i M_i \right] . \tag{A-3}$$

The boundary conditions are the following ($t \geq 0$). For $x = -\infty$;

$$T = T_u \text{ and } Y_i = Y_{iu} \; (i=1,\ldots N) \quad , \tag{A-4}$$

and for $x = \infty$;

$$\frac{\partial T}{\partial x} = \frac{\partial Y_i}{\partial x} = 0 \; (i=1,\ldots N) \quad . \tag{A-5}$$

The transport properties that we are interested in are the diffusion velocities V_i and the heat flux q.

APPENDIX B. H_2-O_2-N_2 INPUT PARAMETERS

The required input data for the H_2-O_2-N_2 flames are for the most part taken from Warnatz (see reference 18 of text).

The kinetic scheme consists of thirty reactions and has been taken in toto from Warnatz' Table 3, which for the most part was taken from the Leeds review.[1] Our interest here is a study of the effects of using different transport algorithms, and not a critical evaluation of the kinetics. So we have uncritically used Warnatz' mechanism. This mechanism is in reasonable agreement with experimental data.

The enthalpies and heat capacities are evaluated using the sixth order polynomial fits of Gordon and McBride (see reference 4 of text). These reproduce the JANNAF (see reference 3 of text) values to within a few parts per thousand over the temperature range 300K-3000K.

The transport parameters are given in Table B-2. These are from Warnatz except for ξ_{ii}^{∞} for OH, which is from Dixon-Lewis (see reference 12 of text). The values for σ and ε/k are obtained from viscosity measurements.

The manipulation of these parameters is discussed in Appendix D.

[B1] *D. L. Baulch, D. D. Drysdale, D. G. Horne, and A. C. Lloyd, Evaluated Kinetic Data for High Temperature Reactions, Vol. 1, Butterworths, London 1972.*

TABLE B-1. REACTIONS IN THE H_2-O_2-N_2 SYSTEM

NO	REACTION	A*	B	C
1	$OH + H_2 \rightarrow H_2O + H$	2.2E13**	0	- 2590
2	$H + H_2O \rightarrow OH + H_2$	9.3E13	0	-10250
3	$H + O_2 \rightarrow OH + O$	2.2E14	0	- 8450
4	$O + OH \rightarrow H + O_2$	1.0E13	0	0
5	$O + H_2 \rightarrow OH + H$	1.8E10	1	- 4480
6	$H + OH \rightarrow O + H_2$	8.3E09	1	- 3500
7	$OH + OH \rightarrow H_2O + O$	6.3E12	0	- 550
8	$O + H_2O \rightarrow OH + OH$	6.8E13	0	- 9240
9	$H + H + M' \rightarrow H_2 + M'$	9.0E17	-1	0
10	$H + OH + M' \rightarrow H_2O + M'$	2.2E22	-2	0
11	$H + O_2 + M' \rightarrow HO_2 + M'$	5.0E15	0	500
12	$H + HO_2 \rightarrow OH + OH$	2.5E14	0	- 950
13	$H + HO_2 \rightarrow H_2 + O_2$	2.5E13	0	- 350
14	$H + HO_2 \rightarrow H_2O + O$	1.5E13	0	- 500
15	$OH + HO_2 \rightarrow H_2O + O_2$	5.0E13	0	- 500
16	$O + HO_2 \rightarrow OH + O_2$	5.0E12	0	- 500
17	$OH + OH + M \rightarrow H_2O_2 + M$	9.1E14	0	2550
18	$H + H_2O_2 \rightarrow H_2O + OH$	3.2E14	0	- 4500
19	$HO_2 + HO_2 \rightarrow H_2O_2 + O_2$	8.5E12	0	- 500
20	$H_2 + M' \rightarrow H + H + M'$	8.8E14	0	-48300
21	$O + O + M \rightarrow O_2 + M$	7.0E13	0	900
22	$HO_2 + M' \rightarrow H + O_2 + M'$	7.0E15	0	-23000
23	$OH + OH \rightarrow HO_2 + H$	1.2E13	0	-20200

TABLE B-1. REACTIONS IN THE H_2-O_2-N_2 SYSTEM (Cont'd)

NO	REACTION	A*	B	C
24	$HO_2 + H_2 \rightarrow H_2O_2 + H$	7.3E11	0	- 9400
25	$H + H_2O_2 \rightarrow H_2 + HO_2$	1.7E12	0	- 1900
26	$H_2O_2 + M \rightarrow OH + OH + M$	1.2E17	0	-22900
27	$O + H_2O_2 \rightarrow OH + HO_2$	2.8E13	0	- 3200
28	$O + H_2O_2 \rightarrow H_2O + O_2$	2.8E13	0	- 3200
29	$OH + H_2O_2 \rightarrow H_2O + HO_2$	1.0E13	0	- 910
30	$HO_2 + H_2O \rightarrow H_2O_2 + OH$	2.8E13	0	-16500

[M] = total concentration

$[M'] = 6.0\,[H_2O] + 1.0\,[H_2] + 0.4\,[O_2] + 0.4\,[N_2]$

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*A is in units of cm^3/mole-sec or cm^6/$mole^2$-sec, $k = AT^B \exp(C/T)$.

**$2.2E13 = 2.2 \times 10^{13}$.

TABLE B-2. MOLECULAR PARAMETERS USED FOR THE DETERMINATION OF TRANSPORT PROPERTIES

Species	σ[Å]	$\frac{\varepsilon}{k}$ [K]	μ[Debye]	α[Å^3]	ξ_{ii}^{∞}
O	2.75	80	0	0	
O_2	3.46	107	0	1.60	14.4
H	2.05	145	0	0	
H_2	2.92	38	0	0.79	280
OH	2.75	80	0	0	4.5
H_2O	2.60	572	1.844	0	4.0
N_2	3.62	97.5	0	0	15.7

HO_2, H_2O_2 like O_2

APPENDIX C. DEFINITION OF THE MATRIX L

The matrix L can be partitioned into nine N by N matrices

$$L = \begin{pmatrix} L^{00,00} & L^{00,10} & L^{00,01} \\ L^{10,00} & L^{10,10} & L^{10,01} \\ L^{01,00} & L^{01,10} & L^{01,01} \end{pmatrix} \tag{C-1}$$

where

$$L_{ii}^{00,00} = 0, \tag{C-2}$$

$$L_{ij}^{00,00} = \frac{16}{25}\frac{T}{P}\left[\frac{X_i X_j}{\mathcal{D}_{ij}} + \sum_{k\neq i} \frac{M_j}{M_i}\frac{X_k X_j}{\mathcal{D}_{ik}}\right], \; i \neq j, \tag{C-3}$$

$$L_{ij}^{00,10} = -\frac{8T}{5P}\,\frac{M_i(1.2\,C_{ij}^{*} - 1)X_i X_j}{(M_i + M_j)\;\mathcal{D}_{ij}}, \; i \neq j, \tag{C-4}$$

$$L_{ii}^{00,10} = -\sum_{j\neq i} L_{ji}^{00,10}, \tag{C-5}$$

$$L_{ij}^{10,00} = L_{ji}^{00,10}, \tag{C-6}$$

$$L_{ij}^{01,00} = L_{ij}^{00,01} = 0 \tag{C-7}$$

$$L_{ii}^{10,10} = -\frac{16\,M_i\,X_i^2}{15\,R\,\eta_i}\left(1 + \frac{10\,C_{i,rot}}{3\pi\,R\,\xi_{ii}}\right) - \frac{16T}{25P}\sum_{k\neq i}\left\{\frac{X_i X_k}{(M_i + M_k)^2\,\mathcal{D}_{ik}} \times \left[\frac{15}{2}M_i^2 + \frac{25}{4}M_k^2 - 3M_k^2\,B_{ik}^{*} + 4M_i M_k A_{ik}^{*}\left(1 + \frac{5}{3\pi}\left\{\frac{C_{i,rot}}{R\,\xi_{ik}} + \frac{C_{k,rot}}{R\,\xi_{ik}}\right\}\right)\right]\right\}, \tag{C-8}$$

$$L_{ij}^{10,10} = \frac{16T}{25P} \frac{M_i M_j \; X_i X_j}{(M_i + M_j)^2 \; \mathcal{D}_{ij}}$$

$$\left\{ \frac{55}{4} - 3 \, B_{ij}^{*} - 4 \, A_{ij}^{*} \left[1 + \right. \right.$$

$$\left. \left. \frac{5}{3\pi} \left(\frac{C_{i,\, rot}}{R \; \xi_{ij}} + \frac{C_{j,\, rot}}{R \; \xi_{ji}} \right) \right] \right\} , \quad i \neq j \qquad \text{(C-9)}$$

$$L_{ii}^{10,01} = \frac{16 M_i \; X_i^{\,2} \; C_{i,\, rot}}{3\pi \; R \; \eta_i \; C_{i,\, int} \; \xi_{ii}}$$

$$+ \frac{32 \; T}{5\pi \; p \; C_{i,\, int}} \sum_{k=i} \frac{M_i \; A^{*}_{ik} \; X_i X_k \; C_{i,\, rot}}{(M_i + M_k) \; \mathcal{D}_{ik} \; \xi_{ik}} , \qquad \text{(C-10)}$$

$$L_{ij}^{10,01} = \frac{32 \; T \; M_j \; A^{*}_{ij} \; X_i \; X_j \; C_{j,\, rot}}{5 \; p \; \pi \; C_{j,\, int} \; (M_i + M_j) \; \mathcal{D}_{ji} \; \xi_{ji}} . \qquad \text{(C-11)}$$

$$L_{ij}^{01,10} = L_{ji}^{10,01} , \qquad \text{(C-12)}$$

$$L_{ij}^{01,10} = 0, \; i \neq j \qquad \text{(C-13)}$$

and

$$L_{ii}^{01,01} = - \frac{8 M_i X_i^{\,2} \; C_{i,\, rot}}{\pi \; \eta_i \; \xi_{ii} \; C_{i,\, int}^{2}}$$

$$- \frac{4RT}{p \; C_{i,\, int}} \left\{ \sum_{k} \frac{X_i X_k}{\mathcal{D}_{i,\, int,k}} \right.$$

$$\left. + \sum_{k \neq i} \frac{12 \; M_i \; A^{*}_{ik} \; X_i X_k \; C_{i,\, rot}}{5\pi \; M_k \; D_{ik} \; C_{i,\, int} \; \xi_{ik}} \right\} . \qquad \text{(C-14)}$$

When solving equations (7) and (6) for the thermal conductivity, λ_o will turn out to have the units cm^2-atm-s^{-1}-K^{-1}. To convert to the more usual units of cal-cm^{-1}-s^{-1}-K^{-1}, we multiply by $R/R_a = 1.9872/82.05$.

APPENDIX D. MANIPULATION OF TRANSPORT DATA

The quantities required to compute the elements of the matrix L used in Method I can be calculated from the transport parameters (Table B-2) and the heat capacities (see reference 4 of text). We shall discuss the procedures in this appendix.

The viscosity η_i and the binary diffusion coefficients $\mathcal{D}_{ij}$ can be obtained from Lennard-Jones (non-polar) or Stockmayer (polar) parameters σ_k and ε_k/k. For polar molecules (here only H_2O) we also need the dipole moment μ_i. For the binary diffusion coefficient of a polar and a non-polar species, we also need the polarizibility α_i of the non-polar species. Then η_i and $\mathcal{D}_{ij}$ are calculated using tabulated values of the collision integrals[1,2] (see also reference 6 of text).

The quantities A^*_{ij}, B^*_{ij}, and C^*_{ij} do not have exactly their standard meanings (see reference 9 of text). However, they can be closely approximated by the usual quotients of collision integrals. For Lennard-Jones parameters, these are tabulated in reference 6 of text. For simplicity, we will assume that at most one of the species is polar (in our case H_2O). Since a polar molecule interacting with a non-polar molecule can be represented by a Lennard-Jones potential, all the quantities A^*_{ij}, B^*_{ij}, and C^*_{ij} can be cast into the Lennard-Jones formalism. They are functions only of $T^*_{ij} = T/(\varepsilon_{ij}/k)$, where ε_{ij} is obtained from ε_i and ε_j by standard combining rules[1] (see also reference 6 of text).

The collision numbers ξ_{ij} for rotational relaxation of species i on colliding with species j are difficult to obtain, particularly if $i \neq j$. Fortunately, these values are not critical. For simplicity, we will assume that $\xi_{ij} = \xi_{ii}$. Parker[3] has calculated values for ξ_{ii} for homonuclear diatomic molecules, as well as the temperature relation

$$\xi_{ii} = \xi^{\infty}_{ii} \left[1 + \frac{\pi^{3/2}}{2(T_i^*)^{1/2}} + \left(\frac{\pi^2}{4} + \pi\right)\frac{1}{T_i^*}\right]^{-1} . \tag{D-1}$$

We use his values for O_2 and N_2. For other types of molecules, we must look for experimental values. In this paper, we take these other ξ_{ii}'s to be constant. The values for ξ_{ii} are taken from Warnatz (see reference 14 of text) except the value of ξ_{ii} for OH (see reference 12 of text).

[D1] *R. C. Reid and T. K. Sherwood, The Properties of Gases and Liquids, 2nd Edition, McGraw-Hill, NY, (1966).*

[D2] *L. Monchick and E. A. Mason, "Transport Properties of Polar Gases", J. Chem. Phys., 33, 1676-1697 (1961).*

The quantities $\mathcal{D}_{i,int,j}$ refer to the diffusion of internal energy, which is approximated by $\mathcal{D}_{ij}$. More accurate values are very difficult to calculate, and there is no known way of determining them experimentally (see reference 9 of text).

To obtain the $C_{i,rot}$ and $C_{i,int}$, we need to properly partition $C_{i,v}$, the heat capacity at constant volume. $C_{i,v}$ can be calculated from the Gordon and McBride polynominal fits (see reference 4 of text). It can be partitioned as

$$C_{i,v} = C_{i,tr} + C_{i,int}, \qquad \text{(D-2)}$$

where $C_{i,tr} = 1.5\ R$. The internal energy can be further partitioned into rotational and vibrational energy. $C_{i,rot} = 0$ for a monatomic molecule, $C_{i,rot} = R$ for a linear molecule, and $C_{i,rot} = 1.5\ R$ for a polyatomic molecule.

For Method I, we do not need to directly compute the separate species thermal conductivities λ_i. These values are required for the other methods, so we will discuss them here.

For monatomic gases,

$$\lambda_i^{mon} = \frac{15}{4} \frac{R}{M_i} \eta_i, \qquad \text{(D-3)}$$

where a hard sphere model has been assumed1 (see also reference 6 of text).

For polyatomic gases, there are many procedures. We will follow the analysis of Mason and Monchick,[1,4] and write

$$\frac{\lambda_i M_i}{\eta_i} = f_{tr}\, C_{i,tr} + f_{int}\, C_{i,int} \qquad \text{(D-4)}$$

where

[D3] *J. G. Parker, "Rotational and Vibrational Relaxation in Diatomic Gases", Phys. Fluids, 2, 449-462 (1959).*

[D4] *E. A. Mason and L. Monchick, "Heat Conductivity of Polyatomic and Polar Gases", J. Chem. Phys., 36, 1622-1639 (1962).*

$$f_{tr} = \frac{5}{2}\left[1 - \frac{10}{3\pi}\left(1 - \frac{2}{5}\ \frac{M_i\ \rho\mathcal{D}_{i,int,i}}{\eta_i}\right)\left(\frac{C_{i,rot}}{R\ \xi_{ii}(rot)}\right.\right.$$

$$\left.\left. + \frac{C_{i,vib}}{R\ \xi_{ii}(vib)}\right)\right] \quad , \qquad \text{(D-5)}$$

$$f_{int} = \frac{M_i\ \rho\mathcal{D}_{i,int,i}}{\eta_i}\left[1 + \frac{5}{\pi}\left(1 - \frac{2}{5}\ \frac{M_i\ \rho\mathcal{D}_{i,int,i}}{\eta_i}\right)\left(\frac{C_{i,rot}}{C_{i,int}\ \xi_{ii}(rot)}\right.\right.$$

$$\left.\left. + \frac{C_{i,vib}}{C_{i,int}\ \xi_{ii}(vib)}\right)\right] . \qquad \text{(D-6)}$$

Normally, $\xi_{ii}(vib) >> \xi_{ii}(rot)$, so we will ignore the vibrational term. We then refer to $\xi_{ii}(rot)$ just as ξ_{ii}. As usual, we approximate $\mathcal{D}_{i,int,i}$ by the self diffusion coefficient $\mathcal{D}_{ii}$.

Using either Lennard-Jones or Stockmayer collision integrals,

$$\frac{M_i\ \rho\mathcal{D}_{ii}}{\eta_i} = 1.1999\ A^* \approx 1.32. \qquad \text{(D-7)}$$

Equation (D-4) then simplifies to

$$\frac{\lambda_i M_i}{\eta_i} = 1.32\ C_{i,v} + 1.77R - .886\ \frac{C_{i,rot}}{\xi_{ii}} \quad . \qquad \text{(D-8)}$$

As before, the exact value of ξ_{ii} is not critical in the computation.

For actual use in the code, a fit to the η_i, λ_i, and $\mathcal{D}_{ij}$ is made of the form aT^b over an appropriate temperature range, using the logarithmic method with proper transformation of weights.[5] The resulting fits are accurate within two percent.

D5 *R. J. Cvetanovic and D. L. Singleton, Internat. J. Chem. Kinet., 9, 481-488, 1977; R. J. Cvetanovic and D. L. Singleton, Internat. J. Chem. Kinet., 1007-1009, 1977.*

The quantities A^*, B^*, and C^* are fit over a range $1.0 \leq T^* \leq 400$. This covers the range likely to occur in a flame. If the fit is extended to values of $T^* \leq 1$, the accuracy suffers. A^* can be fit very accurately by a function of the form: $a(T^*)^b$. To fit B^* and C^* accurately, we need to use the functional form: $a \exp(c/T^*)$ (see Table D-1).

Given the above information, we have developed software to write the actual transport subroutine used in the code.

TABLE D-1. FITS TO THE FUNCTIONS A^*, B^*, C^* ($a(T^*)^b$ or $a \exp(c/T^*)$)

Function	a	b	c
A^*	1.0885	9.0557E-3	0
B^*	1.0786	0	8.5001E-2
C^*	.95426	0	- .14357

APPENDIX E. PROGRAM LISTINGS

We have included here the FORTRAN programs for writing the transport subroutines, as well as examples of the subroutines themselves. Some of these routines are very long for the H_2-O_2-N_2 system (over 3500 lines for Method I). So as an example we have considered a binary mixture of H_2 and N_2. This shows the main features of the programs while conserving space.

A copy of the actual flame code used is given in reference 23 of the text. Method V (constant transport) is included in this code as the default. The appropriate constant transport values for a given flame must be read in, but the subroutine itself is not rewritten.

For our other transport methods, the subroutine is written specifically for a given set of chemical species. The procedure is straightforward. We attach to TAPE15 the coefficients for computing the thermodynamic quantities. We attach to TAPE9 the least squares fits for the viscositites, thermal conductivities, and binary diffusion coefficients. There are computed in another program using the methods discussed in this article. The program also requires the appropriate Lennard-Jones (Stockmayer) parameters, the pressure, and for some methods the least squares fits for A*, B*, and C*. The flame code actually works with non-dimensional forms of the flame equations, so appropriate normalization terms for the space coordinate, time coordinate, and temperature must also be supplied.

The transport statements are written onto TAPE3. This tape is read and attached to a standard set of initial statements. The corresponding FORTRAN subroutine F can then be attached to the flame code.

Given the mass fractions, the non-dimensional temperature, and their first and second space derivatives, F computes the corresponding time derivatives. The needed chemistry terms are found by calling the subroutine RT. This subroutine is also written by a FORTRAN program (see reference 22 of text).

For details on the actual form of the equations used and the connections between F and the rest of the flame code, see reference 23 of the text.

The listing that follows gives the FORTRAN program (MAIN) and the corresponding transport subroutines for a binary mixture of H_2 and N_2 (F) for Methods I, II, III, IV and VI.

```
      PROGRAM LOADF(INPUT,OUTPUT,TAPE5=INPUT,TAPE6=OUTPUT,
     * TAPE3,TAPE9,TAPE15)
C  LOADF CREATES THE SUBROUTINE F IN PDECOL-FLCT.
      DIMENSION II(72)
      DIMENSION LB(25),W(25),AU(7,25),AL(7,25)
      DIMENSION ALD(25),BLD(25),ABD(25,25),BBD(25,25)
      DIMENSION LBPR(25)
      DIMENSION III(44)
      DIMENSION LBROT(25),SGA(25),ESK(25),UM(25),ALP(25),ZROT(25),DF(25)
      DIMENSION LD(25),LDV(25)
      DIMENSION AV(25),BV(25)
      DIMENSION E(25,25)
      WRITE(3,1000)
 1000 FORMAT(1HC,2X,34HWE WANT TO AVOID DIVISION BY ZERO.  )
      WRITE(3,1012)
 1012 FORMAT(6X,14HDO 5 K=1,NPDEM)
      WRITE(3,1014)
 1014 FORMAT(6X,32HIF(ABS(U(K)).LT.SMALL)U(K)=SMALL   )
      WRITE(3,1016)
 1016 FORMAT(1X,1H5,4X,36HIF(ABS(UPH(K)).LT.SMALL)UPH(K)=SMALL   )
      READ(5,12)NLINE
 12   FORMAT(1014)
C  NLINE IS THE NUMBER OF COMMENT LINES TO BE READ AND PRINTED.
      DO 20 K=1,NLINE
      READ(5,22)II
      WRITE(3,22)II
 20   CONTINUE
 22   FORMAT(72A1)
 24   FORMAT(/1X,72A1/)
      READ(5,12)NSPC
      NM=NSPC-1
      LBM=1H-
      LBU=2HU(
      LBP=1H)
      WRITE(3,1020)((LBM,LBU,K,LBP),K=1,NM)
 1020 FORMAT(6X,6HYN=1.0,8(A1,A2,I2,A1),A1,2(/5X,1H*,1X,
     *  8(A2,I2,A1,A1))  )
      WRITE(3,1025)
 1025 FORMAT(6X,33HCALL RT(U,YN,R,NPOE,KPDE,IC,KSKR) )
      WRITE(3,18)NSPC
 18   FORMAT(6X,4HIST=,I2,7H*(IC-1) )
C  ASSUME AT MOST ONE POLAR SPECIES.  (DIPOLE MOMENT NON-ZERO).
C  THEN A* AND B* CAN BE APPROXIMATED BY LENNARD-JONES COLLISION
C  INTEGRALS, EVEN IF THE INPUT PARAMETERS ARE STOCKMAYER.
      DO 30 K=1,NSPC
      READ(5,32)    LB(K),W(K),DF(K),SGA(K),ESK(K),UM(K),ALP(K),ZROT(K),
     * LBROT(K)
      WRITE(6,34)K,LB(K),W(K),DF(K),SGA(K),ESK(K),UM(K),ALP(K),ZROT(K),
     * LBROT(K)
      READ(15,36)(AU(L,K),L=1,5),(III(L),L=1,5)
      WRITE(6,36)(AU(L,K),L=1,5),(III(L),L=1,5)
      READ(15,36)(AU(L,K),L=6,7),(AL(L,K),L=1,3),(III(L),L=1,5)
      WRITE(6,36)(AU(L,K),L=6,7),(AL(L,K),L=1,3),(III(L),L=1,5)
      READ(15,37)(AL(L,K),L=4,7),(III(L),L=1,20)
      WRITE(6,37)(AL(L,K),L=4,7),(III(L),L=1,20)
 30   CONTINUE
      READ(5,232)TPN,PHN,TMN
```

```
232   FORMAT(1P3E12.4)
C  THE ROWS AND COLUMNS CORRESPONDING TO INTERNAL EFFECTS FOR MONATOMICS
C  ARE SKIPPED.  LD KEEPS TRACK OF WHICH ROW OR COLUMN IS BEING
C  WORKED ON.
      LD(1)=1
      IF(DF(1).EQ.0.0)LD(1)=0
      DO 38 L=2,NSPC
      LM=L-1
      LD(L)=LD(LM)+1
      IF(DF(L).EQ.0.0)LD(L)=LD(L)-1
38    CONTINUE
32    FORMAT(A5,7F7.0,A5)
34    FORMAT(/2X,I4,4X,A5,4X,7F8.2,4X,A5/)
36    FORMAT(5E15.8,5A1)
37    FORMAT(4E15.8,20A1)
      WRITE(3,1100)TPN
1100  FORMAT(6X,13HDT=UPH(NPDE)*,1PE14.6)
      WRITE(3,27)
27    FORMAT(6X,22HIF(KSKT.GT.1)GO TO 100)
      WRITE(3,28)
28    FORMAT(6X,22HIF(KSKR.GT.1)GO TO 125   )
      READ(5,12)NLINE
      DO 40 K=1,NLINE
      READ(5,22)II
      WRITE(3,22)II
40    CONTINUE
C  ************************
C  ENTHALPIES AND HEAT CAPACITIES.
C  ************************
      WRITE(3,42)
42    FORMAT(6X,24HIF(T.GT.1000.)GO TO 2000)
      DO 50 K=1,NSPC
      WRITE(3,52)K,AL(1,K),AL(2,K)
      WRITE(3,54)(AL(L,K),L=3,5)
      A=AL(2,K)
      B=AL(3,K)*2.0
      C=AL(4,K)*3.0
      D=AL(5,K)*4.0
      WRITE(3,1112)K,A,B,C,D
1112  FORMAT(6X,2HDC,I2,9H=1.9872*(,1PE16.8,4H+T*(,1PE16.8,/5X,1H*,1X,
     * 2(4H+T*(,1PE16.8),7H)))))*DT )
      WRITE(3,62)K,AL(6,K),AL(1,K)
      WRITE(3,64)AL(2,K),AL(3,K)
      WRITE(3,66)AL(4,K),AL(5,K)
50    CONTINUE
52    FORMAT(6X,1HC,I2,9H=1.9872*(,1PE16.8,4H+T*(,1PE16.8)
54    FORMAT(5X,1H*,1X,3(4H+T*(,1PE16.8),5H)))))
      WRITE(3,56)
56    FORMAT(6X,10HGO TO 3000)
      WRITE(3,58)
58    FORMAT(4H2000,2X,8HCONTINUE)
      DO 60 K=1,NSPC
      WRITE(3,52)K,AU(1,K),AU(2,K)
      WRITE(3,54)(AU(L,K),L=3,5)
      A=AU(2,K)
      B=AU(3,K)*2.0
      C=AU(4,K)*3.0
```

```
      D=AU(5,K)*4.0                                                  MAIN
      WRITE(3,III2)K,A,B,C,D                                         MAIN
      WRITE(3,62)K,AU(6,K),AU(1,K)                                   MAIN
      WRITE(3,64)AU(2,K),AU(3,K)                                     MAIN
      WRITE(3,66)AU(4,K),AU(5,K)                                     MAIN
60    CONTINUE                                                       MAIN
62    FORMAT(6X,1HH,I2,9H=1.9872*(,IPE16.8,4H+T*(,IPEI6.8)           MAIN
64    FORMAT(5X,IH*,IX,4H+I*(,IPEI6.8,4H/2.0,4H+T*(,IPEI6.8,4H/3.0)  MAIN
66    FORMAT(5X,IH*,IX,4H+I*(,IPEI6.8,4H/4.0,4H+T*(,IPEI6.8,         MAIN
     * 4H/5.0,6H))))))                                               MAIN
      WRITE(3,68)                                                    MAIN
68    FORMAT(4H3000,2X,8HCONTINUE)                                   MAIN
      WRITE(3,I34)                                                   MAIN
I34   FORMAT(IHC,2X,39HSPECIFIC HEATS AND SPECIFIC ENTHALPIES.  )    MAIN
      DO I40 K=I,NSPC                                                MAIN
      WRITE(3,I42)K,K,W(K)                                           MAIN
      WRITE(3,II16)K,K,W(K)                                          MAIN
I116  FORMAT(6X,7HDC(IST+,I2,4H)=DC,I2,IH/,F6.2)                     MAIN
      WRITE(3,I44)K,K,W(K)                                           MAIN
I40   CONTINUE                                                       MAIN
I42   FORMAT(6X,6HC(IST+,I2,3H)=C,I2,IH/,F6.2)                       MAIN
I44   FORMAT(6X,6HH(IST+,I2,3H)=H,I2,IH/,F6.2)                       MAIN
      WRITE(3,I46)                                                   MAIN
146   FORMAT(IX,3HI25,2X,8HCONTINUE)                                 MAIN
C  ************************                                          MAIN
C  THERMAL CONDUCTIVITIES AND BINARY DIFFUSION COEFFICIENTS.         MAIN
C  READ IN VISCOSITY, THERMAL CONDUCTIVITY, AND BINARY DIFFUSION     MAIN
C  COEFFICIENTS FROM A FILE CREATED BY VALUES, CY=5.                 MAIN
C  ************************                                          MAIN
      READ(5,I2)NLINE                                                MAIN
      DO 72 K=I,NLINE                                                MAIN
      READ(5,22)II                                                   MAIN
      WRITE(3,22)II                                                  MAIN
72    CONTINUE                                                       MAIN
78    FORMAT(IHC,5X,IHV,I2,IH=,IPEI4.6,5H*(T**,1PEI4.6,IH) )         MAIN
      READ(5,I2)NLINE                                                MAIN
      DO 70 K=I,NLINE                                                MAIN
      READ(5,22)II                                                   MAIN
      WRITE(3,22)II                                                  MAIN
70    CONTINUE                                                       MAIN
      DO 80 K=I,NSPC                                                 MAIN
      READ(9,82)AV(K),BV(K),III                                      MAIN
      WRITE(6,84)K,LB(K),AV(K),BV(K),III                             MAIN
      READ(9,82)ALD(K),BLD(K),III                                    MAIN
      WRITE(6,84)K,LB(K),ALD(K),BLD(K),III                           MAIN
80    CONTINUE                                                       MAIN
82    FORMAT(IP2EI4.6,44AI)                                          MAIN
84    FORMAT(/2X,I4,4X,A4,4X,IP2EI4.6,44AI/)                         MAIN
      DO 76 K=I,NSPC                                                 MAIN
76    WRITE(3,78)K,AV(K),BV(K)                                       MAIN
      DO 90 K=I,NSPC                                                 MAIN
      WRITE(3,92)K,ALD(K),BLD(K)                                     MAIN
90    CONTINUE                                                       MAIN
92    FORMAT(IHC,5X,2HRL,I2,1H=,IPEI4.6,5H*(T**,1PEI4.6,1H) )        MAIN
      READ(5,I2)NLINE                                                MAIN
      DO 100 K=1,NLINE                                               MAIN
      READ(5,22)II                                                   MAIN
```

```
      WRITE(3,22)11
  100 CONTINUE
      NM=NSPC-1
      DO 110 I=1,NSPC
      DO 110 J=I,NSPC
      READ(9,82)ABD(I,J),BBD(I,J),III
      WRITE(6,112)I,J,LB(I),LB(J),ABD(I,J),BBD(I,J),III
  110 CONTINUE
  112 FORMAT(/2X,I4,4X,I4,4X,A4,4X,A4,4X,1P2E14.6,44A1/)
      READ(5,114)PRESS
  114 FORMAT(F6.0)
      WRITE(3,116)PRESS
      WRITE(6,116)PRESS
  116 FORMAT(1HC,2X,7HPRESS =,F6.2)
      DO 120 I=1,NSPC
      DO 120 J=I,NSPC
      ABD(I,J)=ABD(I,J)/PRESS
      WRITE(3,122)I,J,ABD(I,J),BBD(I,J)
  120 CONTINUE
  122 FORMAT(1HC,5X,1HD,2I2,1H=,1PE14.6,5H*(T**,1PE14.6,1H) )
C   ************************
C   SPACE DERIVATIVES.
C   ************************
      LBPL=1H+
      WRITE(3,148)
  148 FORMAT(1HC,2X,42HDEFINE USEFUL COMBINATIONS AND DERIVATIVES )
      NS=NSPC+1
      WRITE(3,149)NS
  149 FORMAT(6X,4HYS=Y,I2)
      DO 150 K=1,NSPC
      WRITE(3,152)K,K
  150 CONTINUE
  152 FORMAT(6X,1HX,I2,2H=Y,I2,3H/YS)
      DO 160 K=1,NM
      WRITE(3,162)K,K
      WRITE(3,164)K,K
      WRITE(3,166)K,K
  160 CONTINUE
  162 FORMAT(6X,1HU,I2,3H=U(,I2,1H))
  164 FORMAT(6X,2HDU,I2,5H=UPH(,I2,1H))
  166 FORMAT(6X,3HDDU,I2,6H=UPH2(,I2,1H))
      LBU=1HU
      WRITE(3,172)NSPC,((LBM,LBU,K),K=1,NM)
  172 FORMAT(6X,1HU,I2,4H=1.0,8(A1,A1,I2),A1,2(/5X,1H*,1X,
     *  8(A1,I2,A1)) )
      LBDU=2HDU
      WRITE(3,174)NSPC,((LBM,LBDU,K),K=1,NM)
  174 FORMAT(6X,2HDU,I2,1H=,8(A1,A2,I2),A1,2(/5X,1H*,1X,
     *  8(A2,I2,A1)) )
      LBDDU=3HDDU
      WRITE(3,176)NSPC,((LBM,LBDDU,K),K=1,NM)
  176 FORMAT(6X,3HDDU,I2,1H=,8(A1,A3,I2),A1,2(/5X,1H*,1X,
     *  8(A3,I2,A1)) )
      DO 180 K=1,NSPC
      WRITE(3,182)K,K,W(K)
  180 CONTINUE
  182 FORMAT(6X,2HDY,I2,3H=DU,I2,1H/,[illegible])
```

```
      LBDY=2HDY
      WRITE(3,186)((LBPL,LBDY,K),K=1,NSPC)
  186 FORMAT(6X,4HDYS=,8(A1,A2,I2),A1,2(/5X,1H*,1X,8(A2,I2,A1)) )
      DO 190 K=1,NSPC
      WRITE(3,188)K,K,W(K)
  188 FORMAT(6X,3HDDY,I2,4H=DDU,I2,1H/,F6.2)
  190 CONTINUE
      LBDDY=3HDDY
      WRITE(3,192)((LBPL,LBDDY,K),K=1,NSPC)
  192 FORMAT(6X,5HDDYS=,5(A1,A3,I2),A1,2(/5X,1H*,1X,5(A3,I2,A1)) )
      PSR=PRESS/82.05
      WRITE(3,234)TPN,PHN,TMN
      WRITE(6,234)TPN,PHN,TMN
  234 FORMAT(1HC,2X,5HTPN =,1PE12.4,6X,5HPHN =,1PE12.4,6X,
     * 5HTMN =,1PE12.4)
      WRITE(3,242)PSR
  242 FORMAT(6X,5HDRH=-,1PE20.12,21H*(DT/T+DYS/YS)/(T*YS) )
      WRITE(3,1202)
 1202 FORMAT(6X,16HDYSY=DYS/(YS*YS) )
      WRITE(3,194)
  194 FORMAT(6X,18HDYSYSQ=(DYS/YS)**2 )
      DO 1250 K=1,NSPC
      WRITE(3,1204)K,K,K
 1204 FORMAT(6X,2HDX,I2,3H=DY,I2,5H/YS-Y,I2,5H*DYSY )
      WRITE(3,196)K,K,K,K,K
  196 FORMAT(6X,3HDDX,I2,5H=(DDY,I2,7H-2.0*DY,I2,13H*DYS/YS+2.0*Y,I2,
     * 9H*DYSYSQ-Y,I2,12H*DDYS/YS)/YS )
C  ZROT HAS BEEN READ IN AT T = INFINITY.
C  IF LBROT = 5H CNST, THEN TREAT ZROT AS A CONSTANT.
C  IF LBROT = 5H  VAR, THEN USE THE FORMULA OF PARKER FOR THE
C  TEMPERATURE DEPENDENCE.
      PI=2.0*ACOS(0.0)
      LBVR=5H  VAR
      LBCN=5H CNST
      IF(DF(K).EQ.0.0)GO TO 1210
      B=SQRT(PI*PI*PI*ESK(K))/2.0
      C=(PI*PI/4.0+PI)*ESK(K)
      A=DF(K)/(2.0*ZROT(K))
      B=A*B
      C=A*C
C  WRITE CROT/ZROT
      IF(LBROT(K).EQ.LBVR)WRITE(3,1206)K,A,B,C
 1206 FORMAT(6X,4HCSZR,I2,1H=,1PE20.12,1H+,1PE20.12,1H/,/5X,1H*,1X,
     * 8HSQRT(T)+,1PE20.12,2H/T )
      IF(LBROT(K).EQ.LBCN)WRITE(3,1207)K,A
 1207 FORMAT(6X,4HCSZR,I2,1H=,1PE20.12)
      B=+B/2.0
      IF(LBROT(K).EQ.LBVR)WRITE(3,1120)K,B,C
 1120 FORMAT(6X,5HDCSZR,I2,3H=-(,1PE19.12,9H/SQRT(T)+,
     * 1PE19.12,8H/T)*DT/T )
      IF(LBROT(K).EQ.LBCN)WRITE(3,1121)K
 1121 FORMAT(6X,5HDCSZR,I2,4H=0.0 )
      A=10.0/(3.0*PI)
      WRITE(3,1274)K,K,A,K
      WRITE(3,1134)K,K,A,K
C  WRITE C INTERNAL.
      A=W(K)/1.9872
```

```
      WRITE(3,1212)K,K,A
 1212 FORMAT(6X,4HCINT,I2,7H=C(IST+,I2,2H)*,1PE20.12,4H-2.5)
      WRITE(3,1124)K,K,A
 1124 FORMAT(6X,5HDCINT,I2,8H=DC(IST+,I2,2H)*,1PE20.12)
      WRITE(3,1216)K,K,K
 1216 FORMAT(6X,3HCSC,I2,5H=CSZR,I2,5H/CINT,I2)
      WRITE(3,1128)K,K,K,K,K
 1128 FORMAT(6X,4HDCSC,I2,7H=(DCSZR,I2,5H-CSZR,I2,6H*DCINT,I2,
     * 5H/CINT,I2,6H)/CINT,I2 )
      GO TO 1250
 1210 CONTINUE
      WRITE(3,1272)K,K
      WRITE(3,1132)K,K
 1250 CONTINUE
      DO 1300 I=1,NSPC
      DO 1300 J=1,NSPC
      WRITE(3,1254)I,J,I,J
 1254 FORMAT(6X,1HX,2I2,2H=X,I2,2H*X,I2)
      WRITE(3,1256)I,J,I,J,I,J
 1256 FORMAT(6X,2HDX,2I2,3H=DX,I2,2H*X,I2,2H+X,I2,3H*DX,I2)
      A=1.0/ABD(I,J)
      B=-BBD(I,J)
C  WRITE THE RECIPROCAL OF THE BINARY DIFFUSION COEFFICIENT.
      WRITE(3,1258)I,J,A,B
 1258 FORMAT(6X,2HVD,2I2,1H=,1PE20.12,6H*(T**(,1PE14.6,2H)) )
      A=A*B
      B=B-1.0
      WRITE(3,1262)I,J,A,B
 1262 FORMAT(6X,3HDVD,2I2,1H=,1PE20.12,6H*(T**(,1PE14.6,5H))*DT )
      WRITE(3,1266)I,J,I,J,I,J
 1266 FORMAT(6X,3HXSD,2I2,2H=X,2I2,3H*VD,2I2)
      WRITE(3,1270)((I,J),L=1,5)
 1270 FORMAT(6X,4HDXSD,2I2,3H=DX,2I2,3H*VD,2I2,2H+X,2I2,4H*DVD,2I2)
      IF(I.EQ.J)GO TO 1300
      A=5.0/(3.0*PI)
      IF(DF(I).EQ.0.0.AND.DF(J).EQ.0.0)WRITE(3,1272)I,J
      IF(DF(I).EQ.0.0.AND.DF(J).EQ.0.0)WRITE(3,1132)I,J
 1132 FORMAT(6X,3HDCZ,2I2,4H=0.0)
 1272 FORMAT(6X,2HCZ,2I2,4H=1.0)
      IF(DF(I).NE.0.0.AND.DF(J).EQ.0.0)WRITE(3,1274)I,J,A,I
      IF(DF(I).NE.0.0.AND.DF(J).EQ.0.0)WRITE(3,1134)I,J,A,I
 1134 FORMAT(6X,3HDCZ,2I2,1H=,1PE20.12,7H*(DCSZR,I2,1H) )
 1274 FORMAT(6X,2HCZ,2I2,5H=1.0+,1PE20.12,6H*(CSZR,I2,1H) )
      IF(DF(I).EQ.0.0.AND.DF(J).NE.0.0)WRITE(3,1274)I,J,A,J
      IF(DF(I).EQ.0.0.AND.DF(J).NE.0.0)WRITE(3,1134)I,J,A,J
      IF(DF(I).NE.0.0.AND.DF(J).NE.0.0)WRITE(3,1276)I,J,A,I,J
      IF(DF(I).NE.0.0.AND.DF(J).NE.0.0)WRITE(3,1136)I,J,A,I,J
 1136 FORMAT(6X,3HDCZ,2I2,1H=,1PE20.12,7H*(DCSZR,I2,6H+DCSZR,I2,1H) )
 1276 FORMAT(6X,2HCZ,2I2,5H=1.0+,1PE20.12,6H*(CSZR,I2,5H+CSZR,I2,1H) )
 1300 CONTINUE
      LBX=1HX
      LBVD=3H*VD
      K=1
      WRITE(3,1304)K,((LBPL,LBX,L,LBVD,K,L),L=2,NSPC)
 1304 FORMAT(6X,4HSXSD,I2,1H=,5(2A1,I2,A3,2I2),A1,3(/5X,1H*,1X,
     * 5(A1,I2,A3,2I2,A1)) )
      LBDX=2HDX
```

```
      LBDVD=4H*DVD                                                     MAIN
      WRITE(3,1308)K,((LBPL,LBDX,L,LBVD,K,L,LBPL,LBX,L,LBDVD,K,L)      MAIN
     * ,L=2,NSPC)                                                      MAIN
 1308 FORMAT(6X,5HDSXSD,I2,1H=,2(A1,A2,I2,A3,2I2,2A1,I2,A4,2I2),A1,    MAIN
     * 9(/5X,1H*,1X,2(A2,I2,A3,2I2,2A1,I2,A4,2I2,A1)) )                MAIN
      DO 1310 K=2,NM                                                   MAIN
      KM=K-1                                                           MAIN
      KP=K+1                                                           MAIN
      WRITE(3,1304)K,((LBPL,LBX,L,LBVD,L,K),L=1,KM),                   MAIN
     * ((LBPL,LBX,L,LBVD,K,L),L=KP,NSPC)                               MAIN
      WRITE(3,1308)K,((LBPL,LBDX,L,LBVD,L,K,LBPL,LBX,L,LBDVD,L,K),     MAIN
     * L=1,KM),((LBPL,LBDX,L,LBVD,K,L,LBPL,LBX,L,LBDVD,K,L),L=KP,NSPC) MAIN
 1310 CONTINUE                                                         MAIN
      K=NSPC                                                           MAIN
      WRITE(3,1304)K,((LBPL,LBX,L,LBVD,L,K),L=1,NM)                    MAIN
      WRITE(3,1308)K,((LBPL,LBDX,L,LBVD,L,K,LBPL,LBX,L,LBDVD,L,K),     MAIN
     * L=1,NM)                                                         MAIN
      DO 1325 K=1,NSPC                                                 MAIN
      A=1.0/AV(K)                                                      MAIN
      B=-BV(K)-1.0                                                     MAIN
C  WRITE THE RECIPROCAL OF THE VISCOSITY TIMES THE TEMPERATURE.        MAIN
      WRITE(3,1312)K,A,B                                               MAIN
 1312 FORMAT(6X,3HSTV,I2,1H=,1PE20.12,6H*(T**(,1PE14.6,2H)) )          MAIN
      A=A*B                                                            MAIN
      B=B-1.0                                                          MAIN
      WRITE(3,1314)K,A,B                                               MAIN
 1314 FORMAT(6X,4HDSTV,I2,1H=,1PE20.12,6H*(T**(,1PE14.6,5H))*DT)       MAIN
      WRITE(3,1316)K,K,K,K                                             MAIN
 1316 FORMAT(6X,4HXSTV,I2,2H=X,2I2,4H*STV,I2)                          MAIN
      WRITE(3,1320)K,K,K,K,K,K,K                                       MAIN
 1320 FORMAT(6X,5HDXSTV,I2,3H=DX,2I2,4H*STV,I2,2H+X,2I2,5H*DSTV,I2)    MAIN
 1325 CONTINUE                                                         MAIN
C  ************************                                            MAIN
C  SPECIFIC HEAT OF THE MIXTURE.                                       MAIN
C  ************************                                            MAIN
      WRITE(3,124)                                                     MAIN
  124 FORMAT(1HC,2X,44HSPECIFIC HEAT OF THE MIXTURE.  NTIS FORMULA. )  MAIN
      LBC=6HC(1ST+                                                     MAIN
      LBU=3H)*U                                                        MAIN
      WRITE(3,132)((LBPL,LBC,K,LBU,K),K=1,NSPC)                        MAIN
  132 FORMAT(6X,7HCM(IC)=,4(A1,A6,I2,A3,I2),A1,                        MAIN
     * 4(/5X,1H*,1X,4(A6,I2,A3,I2,A1)) )                               MAIN
C  ************************                                            MAIN
C  THERMAL CONDUCTIVITY AND DIFFUSION.                                 MAIN
C  ************************                                            MAIN
C  BOLTZMAN CONSTANT.                                                  MAIN
      RK=1.38054E-16                                                   MAIN
C  GAS CONSTANT.                                                       MAIN
      RG=1.9872                                                        MAIN
      WRITE(3,272)                                                     MAIN
      WRITE(3,274)                                                     MAIN
  272 FORMAT(1HC,2X,24HDIFFUSION AND HEAT FLUX.      )                 MAIN
  274 FORMAT(1HC,2X,16HSEE DIXON-LEWIS,    )                           MAIN
      WRITE(3,276)                                                     MAIN
  276 FORMAT(1HC,2X,60H11.  TRANSPORT PHENOMENA IN MULTICOMPONENT SYSTEM MAIN
     *S.                    )                                          MAIN
      READ(5,279)AAST,BAST,111                                         MAIN
```

```
 279   FORMAT(IP2EI4.6,44AI)
       WRITE(6,123)AAST,BAST,III
 123   FORMAT(/2X,IP2EI4.6,44AI)
       READ(5,279)ABST,CBST,III
       WRITE(6,123)ABST,CBST,III
       READ(5,279)ACST,CCST,III
       WRITE(6,123)ACST,CCST,III
C  LM 00,00
       WRITE(3,30I)
 30I   FORMAT(IHC,2X,8HLM 00,00)
       DO 305 K=I,NSPC
       WRITE(3,302)K,K
 305   CONTINUE
 302   FORMAT(6X,2HZ(,I2,IH,,I2,5H)=0.0   )
       DO 310 I=1,NSPC
       DO 310 J=1,NSPC
       IF(I.EQ.J)GO TO 310
       A =W(J)/W(I)
       IMIN=MIN0(I,J)
       IMAX=MAX0(I,J)
       WRITE(3,308)I,J,IMIN,IMAX,A,J,I
 308   FORMAT(6X,2HZ(,I2,IH,,I2,5H)=X5D,2I2,IH+,IPE20.I2,2H*X,I2,
      * 5H*SXSD,I2)
       WRITE(3,312)I,J,IMIN,IMAX,A,J,I,J,I
 312   FORMAT(6X,2HDZ,I2,IHS,I2,5H=DXSD,2I2,1H+,IPE20.I2,4H*(DX,I2,
      * 5H*SXSD,I2,2H+X,I2,6H*DSXSD,I2,1H) )
 310   CONTINUE
C  FIND THE SIGMA FOR EACH PAIR OF SPECIES.
C  ASSUME THAT ONLY ONE SPECIES IS POLAR.
       DO 320 I=I,NSPC
       DO 320 J=I,NSPC
       IF(I.EQ.J)GO TO 320
       E(I,J)=SQRT(ESK(I)*ESK(J))
       IF(UM(I).EQ.0.0.AND.UM(J).EQ.0.0)GO TO 320
C  COMBINING RULE.  P. 528, REID AND SHERWOOD.
       IF(UM(I).NE.0.0)LP=I
       IF(UM(J).NE.0.0)LP=J
       IF(LP.EQ.I)LNP=J
       IF(LP.EQ.J)LNP=I
       UMP=UM(LP)*1.0E-I8
       SGC=SGA(LP)*1.0E-8
       TPSTAR=UMP*UMP/(ESK(LP)*RK*SGC*SGC*SGC*SQRT(8.0))
       FC=I.0+(I.0/SQRT(2.0))*(ALP(LNP)*TPSTAR/(SGA(LNP)**3))*
      * SQRT(ESK(LP)/ESK(LNP))
       WRITE(6,1234)I,J,LP,LNP,FC
 I234  FORMAT(4I4,IPE12.4)
       E(I,J)=E(I,J)*FC*FC
 320   CONTINUE
C  FIND T*, A*, B*, AND C*.
       WRITE(3,1350)
 1350  FORMAT(IHC,2X,24HFIND T*, A*, B*, AND C*.    )
       DO 1360 I=I,NM
       IP=I+I
       DO 1360 J=IP,NSPC
       WRITE(3,1354)E(I,J)
 1354  FORMAT(6X,5HTS=T/,1PE14.6)
       WRITE(3,1364)E(I,J)
```

```
 1364 FORMAT(6X,7HDTS=DT/,1PE14.6)
      WRITE(3,1356)I,J,AAST,BAST
 1356 FORMAT(6X,3HAST,2I2,1H=,1PE14.6,7H*(TS**(,1PE14.6,2H)) )
      A=AAST*BAST
      B=BAST-1.0
      WRITE(3,1366)I,J,A,B
 1366 FORMAT(6X,4HDAST,2I2,1H=,1PE20.12,11H*DTS*(TS**(,1PE14.6,2H)) )
      WRITE(3,1365)CBST
 1365 FORMAT(6X,7HEX=EXP(,1PE14.6,4H/TS) )
      LBB=3HBST
      WRITE(3,1358)LBB,I,J,ABST
 1358 FORMAT(6X,A3,2I2,1H=,1PE14.6,3H*EX)
      LBDB=4HDBST
      A=-ABST*CBST
      WRITE(3,1368)LBDB,I,J,A
 1368 FORMAT(6X,A4,2I2,1H=,1PE14.6,15H*DTS*EX/(TS*TS) )
      WRITE(3,1365)CCST
      LBC=3HCST
      WRITE(3,1358)LBC,I,J,ACST
      LBDC=4HDCST
      A=-ACST*CCST
      WRITE(3,1368)LBDC,I,J,A
 1360 CONTINUE
C  LM 00,10 AND LM 10,00
      WRITE(3,321)
 321  FORMAT(1HC,2X,21HLM 00,10 AND LM 10,00 )
      DO 330 IS=1,NSPC
      DO 330 JS=1,NSPC
      IF(IS.EQ.JS)GO TO 330
      I=IS
      J=JS+NSPC
      A=-2.5*W(IS)/(W(IS)+W(JS))
      IMIN=MIN0(IS,JS)
      IMAX=MAX0(IS,JS)
      WRITE(3,326)A,IMIN,IMAX
 326  FORMAT(6X,3HCT=,1PE20.12,9H*(1.2*CST,2I2,5H-1.0) )
      A=A*1.2
      WRITE(3,1140)A,IMIN,IMAX
 1140 FORMAT(6X,4HDCT=,1PE20.12,5H*DCST,2I2)
      IMIN=MIN0(IS,JS)
      IMAX=MAX0(IS,JS)
      WRITE(3,328)I,J,IMIN,IMAX
 328  FORMAT(6X,2HZ(,I2,1H,,I2,8H)=CT*XSD,2I2)
      WRITE(3,1144)I,J,IMIN,IMAX,IMIN,IMAX
 1144 FORMAT(6X,2HDZ,I2,1HS,I2,8H=CT*DXSD,2I2,8H+DCT*XSD,2I2)
 330  CONTINUE
      I1=1
      I2=1+NSPC
      LBZ=2HZ(
      LBC=1H,
      LBP=1H)
      LBM=1H-
      WRITE(3,336)I1,I2,((LBM,LBZ,K,LBC,I2,LBP),K=2,NSPC)
 336  FORMAT(6X,2HZ(,I2,1H,,I2,2H)=,5(A1,A2,I2,A1,I2,A1),A1,
     * 3(/5X,1H*,1X,5(A2,I2,A1,I2,2A1)) )
      LBDZ=2HDZ
      LBSP=1HS
```

```
      WRITE(3,338)II,I2,((LBM,LBDZ,K,LHSP,I2),K=2,NSPC)
338   FORMAT(6X,2HDZ,I2,1HS,I2,IH=,4(A1,A2,I2,AI,I2),A1,
     * 2(/5X,1H*,IX,7(A2,12,AI,I2,A1)) )
      DO 340 I=2,NM
      IM=I-I
      IP=I+I
      I1=I
      I2=I+NSPC
      WRITE(3,336)II,I2,((LBM,LBZ,K,LHC,I2,LBP),K=I,IM),
     * ((LBM,LBZ,K,LBC,I2,LBP),K=IP,NSPC)
      WRITE(3,338)II,12,((LBM,LBDZ,K,LBSP,I2),K=I,IM),
     * ((LBM,LBDZ,K,LBSP,12),K=IP,NSPC)
340   CONTINUE
      II=NSPC
      I2=NSPC+NSPC
      WRITE(3,336)II,I2,((LBM,LBZ,K,LHC,I2,LBP),K=I,NM)
      WRITE(3,338)1I,I2,((LBM,LBDZ,K,LBSP,I2),K=I,NM)
      DO 350 IS=I,NSPC
      DO 350 JS=I,NSPC
      IN=IS+NSPC
      JN=JS
      WRITE(3,342)IN,JN,JN,IN
      WRITE(3,346)IN,JN,JN,IN
342   FORMAT(6X,2HZ(,I2,IH,,I2,4H)=Z(,12,IH,,I2,IH) )
346   FORMAT(6X,2HDZ,I2,IHS,I2,3H=DZ,I2,IHS,I2)
350   CONTINUE
C  LM 0I,00 AND LM 00,0I
C  ROWS OF LM 0I,00 AND COLUMNS OF LM 00,0I CORRESPONDING TO
C  MONATOMICS ARE DELETED.
      WRITE(3,35I)
35I   FORMAT(IHC,2X,2IHLM 0I,00 AND LM 00,0I )
      DO 360 IS=I,NSPC
      DO 360 JS=I,NSPC
      IF(DF(IS).EQ.0.0)GO TO 360
      I=LD(IS)+2*NSPC
      J=JS
      WRITE(3,362)I,J
362   FORMAT(6X,2HZ(,I2,1H,,I2,5H)=0.0)
360   CONTINUE
      DO 363 IS=1,NSPC
      DO 363 JS=I,NSPC
      IF(DF(JS).EQ.0.0)GO TO 363
      I=IS
      J=LD(JS)+2*NSPC
      WRITE(3,362)I,J
363   CONTINUE
C  LM 10,I0   SYMMETRIC.
      WRITE(3,361)
361   FORMAT(1HC,2X,8HLM I0,I0 )
      DO 370 IS=1,NM
      IP=IS+1
      DO 370 JS=IP,NSPC
      I=IS+NSPC
      J=JS+NSPC
      A=W(IS)*W(JS)/((W(IS)+W(JS))**2)
      WRITE(3,372)A,IS,JS,IS,JS,IS,JS
372   FORMAT(6X,3HCT=,1PE20.12,15H*(13.75-3.0*ASI,2I2,
```

```
       * 8H-4.0*AST,2I2,3H*CZ,2I2,1H) )
         WRITE(3,1146)A,IS,JS,IS,JS,IS,JS,IS,JS,IS,JS
  1146   FORMAT(6X,5HDCT=-,1PE20.12,10H*(3.0*DBST,2I2,9H+4.0*(AST,
       * 2I2,4H*DCZ,2I2,/5X,1H*,1X,5H+DAST,2I2,3H*CZ,2I2,2H)) )
         WRITE(3,376)I,J,IS,JS
   376   FORMAT(6X,2HZ(,I2,1H,,I2,8H)=CT*XSD,2I2)
         WRITE(3,377)J,I,I,J
   377   FORMAT(6X,2HZ(,I2,1H,,I2,4H)=Z(,I2,1H,,I2,1H) )
         WRITE(3,380)I,J,IS,JS,IS,JS
   380   FORMAT(6X,2HDZ,I2,1HS,I2,8H=CT*DXSD,2I2,8H+DCT*XSD,2I2)
         WRITE(3,379)J,I,I,J
   379   FORMAT(6X,2HDZ,I2,1HS,I2,3H=DZ,I2,1HS,I2)
   370   CONTINUE
         DO 400 IS=1,NSPC
         I=IS+NSPC
         RGA=82.05
C  USE THE GAS CONSTANT IN UNITS OF CM**3-ATM/MOLE-K SO ALL THE
C  ELEMENTS OF Z ARE IN THE SAME UNITS.
         A=-5.0*PRESS*W(IS)/(3.0*RGA)
         WRITE(3,382)A,IS,IS
   382   FORMAT(6X,3HCT=,1PE20.12,3H*CZ,2I2)
         WRITE(3,383)A,IS,IS
   383   FORMAT(6X,4HDCT=,1PE20.12,4H*DCZ,2I2)
         DO 390 KS=1,NSPC
         IF(KS.EQ.IS)GO TO 390
         IMIN=MIN0(IS,KS)
         IMAX=MAX0(IS,KS)
         A=7.5*W(IS)*W(IS)+6.25*W(KS)*W(KS)
         B=3.0*W(KS)*W(KS)
         C=4.0*W(IS)*W(KS)
         RMT=1.0/((W(IS)+W(KS))**2)
         A=A*RMT
         B=B*RMT
         C=C*RMT
         WRITE(3,386)KS,C,IMIN,IMAX,IMIN,IMAX
   386   FORMAT(6X,2HCT,I2,1H=,1PE20.12,4H*AST,2I2,3H*CZ,2I2)
         WRITE(3,1150)KS,C,((IMIN,IMAX),L=1,4)
  1150   FORMAT(6X,3HDCT,I2,1H=,1PE20.12,6H*(DAST,2I2,3H*CZ,2I2,
       * 4H+AST,2I2,4H*DCZ,2I2,1H) )
         WRITE(3,388)KS,A,B,IMIN,IMAX,KS
   388   FORMAT(6X,2HCT,I2,1H=,1PE20.12,1H-,1PE20.12,4H*BST,2I2,3H+CT,I2)
         WRITE(3,1154)KS,B,IMIN,IMAX,KS
  1154   FORMAT(6X,3HDCT,I2,2H=-,1PE20.12,5H*DBST,2I2,4H+DCT,I2)
   390   CONTINUE
         LBXSD=3HXSD
         LBDXSD=4HDXSD
         LBCT=3H*CT
         LBDCT=4H*DCT
         IF(IS.GT.1)GO TO 393
         WRITE(3,392)I,I,IS,((LBM,LBXSD ,IS,KS,LBCT,KS),KS=2,NSPC)
   392   FORMAT(6X,2HZ(,I2,1H,,I2,9H)=CT*XSTV,I2,
       * 2(A1,A3,2I2,A3,I2),A1,5(/5X,1H*,1X,4(A3,2I2,A3,I2,A1)) )
         WRITE(3,394)I,I,IS,IS,((LBM,LBDXSD,IS,KS,LBCT,KS,LBM,LBXSD,IS,
       * KS,LBDCT,KS),KS=2,NSPC)
   394   FORMAT(6X,2HDZ,I2,1HS,I2,9H=CT*DXSTV,I2,9H+DCT*XSTV,I2,A1,A4,
       * 2I2,A3,I2,A1,A3,2I2,A4,I2,A1,I0(/5X,1H*,1X,2(A4,2I2,A3,I2,A1,A3,
       * 2I2,A4,I2,A1)) )
```

```
      GO TO 400                                                          MAIN
  393 IF(IS.LT.NSPC)GO TO 396                                            MAIN
      WRITE(3,392)I,I,IS,((LBM,LBXSD ,KS,IS,LBCT,KS),KS=1,NM)            MAIN
      WRITE(3,394)I,I,IS,IS,((LBM,LBDXSD,KS,IS,LBCT,KS,LBM,LBXSD,        MAIN
     * KS,IS,LBDCT,KS),KS=1,NM)                                          MAIN
      GO TO 400                                                          MAIN
  396 IM=IS-1                                                            MAIN
      IP=IS+1                                                            MAIN
      WRITE(3,392)I,I,IS,((LBM,LBXSD ,KS,IS,LBCT,KS),KS=1,IM),           MAIN
     * ((LBM,LBXSD ,IS,KS,LBCT,KS),KS=IP,NSPC)                           MAIN
      WRITE(3,394)I,I,IS,IS,((LBM,LBDXSD,KS,IS,LBCT,KS,LBM,LBXSD,KS,IS,  MAIN
     * LBDCT,KS),KS=1,IM),((LBM,LBDXSD,IS,KS,LBCT,KS,LBM,LBXSD,IS,KS,    MAIN
     * LBDCT,KS),KS=IP,NSPC)                                             MAIN
  400 CONTINUE                                                           MAIN
C  LM 10,01 AND LM 01,10                                                 MAIN
C  ROWS OF LM 01,10 AND COLUMNS OF LM 10,01 CORRESPONDING TO MONATOMICS  MAIN
C  ARE ELIMINATED.                                                       MAIN
      WRITE(3,401)                                                       MAIN
  401 FORMAT(1HC,2X,21HLM 10,01 AND LM 01,10 )                           MAIN
      DO 420 IS=1,NSPC                                                   MAIN
      DO 420 JS=1,NSPC                                                   MAIN
      IF(IS.EQ.JS)GO TO 420                                              MAIN
      IF(DF(JS).EQ.0.0)GO TO 420                                         MAIN
      IMIN=MIN0(IS,JS)                                                   MAIN
      IMAX=MAX0(IS,JS)                                                   MAIN
      I=IS+NSPC                                                          MAIN
      J=LD(JS)+2*NSPC                                                    MAIN
      A=10.0*W(JS)/(PI*(W(IS)+W(JS)))                                    MAIN
      WRITE(3,402)A,IMIN,IMAX,JS                                         MAIN
  402 FORMAT(6X,3HCT=,1PE20.12,4H*AST,2I2,4H*CSC,2I2)                    MAIN
      WRITE(3,1156)A,IMIN,IMAX,JS,IMIN,IMAX,JS                           MAIN
 1156 FORMAT(6X,4HDCT=,1PE20.12,6H*(DAST,2I2,4H*CSC,I2,4H+AST,2I2,       MAIN
     * 5H*DCSC,I2,1H) )                                                  MAIN
      WRITE(3,404)I,J,IMIN,IMAX                                          MAIN
  404 FORMAT(6X,2HZ(,I2,1H,,I2,5H)=XSD,2I2,3H*CT)                        MAIN
      WRITE(3,408)I,J,IMIN,IMAX,IMIN,IMAX                                MAIN
  408 FORMAT(6X,2HDZ,I2,1HS,I2,5H=DXSD,2I2,7H*CT+XSD,2I2,4H*DCT )        MAIN
  420 CONTINUE                                                           MAIN
      DO 450 IS=1,NSPC                                                   MAIN
      IF(DF(IS).EQ.0.0)GO TO 450                                         MAIN
      I=IS+NSPC                                                          MAIN
      J=LD(IS)+2*NSPC                                                    MAIN
      A=25.0*PRESS*W(IS)/(3.0*PI*RGA)                                    MAIN
      WRITE(3,422)A,IS                                                   MAIN
  422 FORMAT(6X,3HCT=,1PE20.12,4H*CSC,I2)                                MAIN
      WRITE(3,1160)A,IS                                                  MAIN
 1160 FORMAT(6X,4HDCT=,1PE20.12,5H*DCSC,I2)                              MAIN
      DO 430 KS=1,NSPC                                                   MAIN
      IF(KS.EQ.IS)GO TO 430                                              MAIN
      A=10.0*W(IS)/(PI*(W(IS)+W(KS)))                                    MAIN
      IMIN=MIN0(IS,KS)                                                   MAIN
      IMAX=MAX0(IS,KS)                                                   MAIN
      WRITE(3,426)KS,A,IMIN,IMAX,IS                                      MAIN
      WRITE(3,1162)KS,A,IMIN,IMAX,IS,IMIN,IMAX,IS                        MAIN
 1162 FORMAT(6X,3HDCT,I2,1H=,1PE20.12,6H*(DAST,2I2,4H*CSC,I2,            MAIN
     * 4H+AST,2I2,5H*DCSC,I2,1H) )                                       MAIN
  426 FORMAT(6X,2HCT,I2,1H=,1PE20.12,4H*AST,2I2,4H*CSC,I2)               MAIN
```

```
 430  CONTINUE
      LBCT=2HCT
      LBDCT=3HDCT
      LBXSD=4H*XSD
      LBDXSD=5H*DXSD
      IF(IS.GT.1)GO TO 433
      WRITE(3,432)I,J,IS,((LBPL,LBCT,KS,LBXSD ,IS,KS),KS=2,NSPC)
 432  FORMAT(6X,2HZ(,I2,1H,,I2,9H)=CT*XSTV,I2,3(A1,A2,I2,A4,2I2),A1,
     * 5(/5X,1H*,1X,4(A2,I2,A4,2I2,A1)) )
      WRITE(3,434)I,J,IS,IS,((LBPL,LBCT,KS,LBDXSD,IS,KS,LBPL,LBDCT,
     * KS,LBXSD,IS,KS),KS=2,NSPC)
 434  FORMAT(6X,2HDZ,I2,1HS,I2,9H=CT*DXSTV,I2,9H+DCT*XSTV,I2,
     * A1,A2,I2,A5,2I2,A1,A3,I2,A4,2I2,A1,10(/5X,1H*,1X,
     * 2(A2,I2,A5,2I2,A1,A3,I2,A4,2I2,A1)) )
      GO TO 440
 433  IF(IS.LT.NSPC)GO TO 436
      WRITE(3,432)I,J,IS,((LBPL,LBCT,KS,LBXSD ,KS,IS),KS=1,NM)
      WRITE(3,434)I,J,IS,IS,((LBPL,LBCT,KS,LBDXSD,KS,IS,LBPL,LBDCT,
     * KS,LBXSD,KS,IS),KS=1,NM)
      GO TO 440
 436  CONTINUE
      IM=IS-1
      IP=IS+1
      WRITE(3,432)I,J,IS,((LBPL,LBCT,KS,LBXSD ,KS,IS),KS=1,IM),
     * ((LBPL,LBCT,KS,LBXSD ,IS,KS),KS=IP,NSPC)
      WRITE(3,434)I,J,IS,IS,((LBPL,LBCT,KS,LBDXSD,KS,IS,LBPL,LBDCT,
     * KS,LBXSD,KS,IS),KS=1,IM),((LBPL,LBCT,KS,LBDXSD,IS,KS,LBPL,LBDCT,
     * KS,LBXSD,IS,KS),KS=IP,NSPC)
 440  CONTINUE
 450  CONTINUE
      DO 418 IS=1,NSPC
      DO 418 JS=1,NSPC
      IF(DF(IS).EQ.0.0)GO TO 418
      I=LD(IS)+2*NSPC
      J=JS+NSPC
      WRITE(3,412)I,J,J,I
 412  FORMAT(6X,2HZ(,I2,1H,,I2,4H)=Z(,I2,1H,,I2,1H) )
      WRITE(3,416)I,J,J,I
 416  FORMAT(6X,2HDZ,I2,1HS,I2,3H=DZ,I2,1HS,I2)
 418  CONTINUE
C  LM 01,01
C  ROWS AND COLUMNS OF LM 01,01 CORRESPONDING TO MONATOMICS ARE DELETED.
      WRITE(3,451)
 451  FORMAT(1HC,2X,8HLM 01,01 )
      DO 460 IS=1,NSPC
      DO 460 JS=1,NSPC
      IF(IS.EQ.JS)GO TO 460
      IF(DF(IS).EQ.0.0.OR.DF(JS).EQ.0.0)GO TO 460
      I=LD(IS)+2*NSPC
      J=LD(JS)+2*NSPC
      WRITE(3,362)I,J
 460  CONTINUE
      LBBL=1H
      LBP=1H)
      DO 490 IS=1,NSPC
      IF(DF(IS).EQ.0.0)GO TO 490
      I=LD(IS)+2*NSPC
```

```
      WRITE(3,462)IS
  462 FORMAT(6X,14HCTM=-6.25/CINT,I2)
      WRITE(3,1166)IS,IS,IS
 1166 FORMAT(6X,15HDCTM=6.25*DCINT,I2,6H/(CINT,I2,5H*CINT,I2,1H) )
      A=2.0*PRESS*W(IS)/(PI*RGA)
      WRITE(3,466)A,IS
  466 FORMAT(6X,3HCT=,1PE20.12,4H*CSC,I2)
      WRITE(3,1170)A,IS
 1170 FORMAT(6X,4HDCT=,1PE20.12,5H*DCSC,I2)
      DO 470 KS=1,NSPC
      IF(IS.EQ.KS)GO TO 470
      A=12.0*W(IS)/(5.0*PI*W(KS))
      IMIN=MIN0(IS,KS)
      IMAX=MAX0(IS,KS)
      WRITE(3,472)KS,A,IMIN,IMAX,IS
  472 FORMAT(6X,2HCT,I2,5H=1.0+,1PE20.12,4H*AST,2I2,4H*CSC,I2)
      WRITE(3,1172)KS,A,IMIN,IMAX,IS,IMIN,IMAX,IS
 1172 FORMAT(6X,3HDCT,I2,1H=,1PE20.12,6H*(DAST,2I2,4H*CSC,I2,
     * 4H+AST,2I2,5H*DCSC,I2,1H) )
  470 CONTINUE
      IF(IS.GT.1)GO TO 475
      WRITE(3,1176)IS,IS,IS,((LBPL,LBCT,KS,LBXSD,IS,KS),KS=2,NSPC)
 1176 FORMAT(6X,4HSUM=,7HCT*XSTV,I2,4H+XSD,2I2,2(A1,A2,I2,A4,2I2),A1,
     * 5(/5X,1H*,1X,4(A2,I2,A4,2I2,A1)) )
      WRITE(3,1180)IS,IS,IS,IS,((LBPL,LBCT,KS,LBDXSD,IS,KS,LBPL,LBDCT,
     * KS,LBXSD,IS,KS),KS=2,NSPC)
 1180 FORMAT(6X,5HDSUM=,8HDCT*XSTV,I2,9H+CT*DXSTV,I2,5H+DXSD,2I2,
     * A1,A2,I2,A5,2I2,A1,A3,I2,A4,2I2,A1,10(/5X,1H*,1X,
     * 2(A2,I2,A5,2I2,A1,A3,I2,A4,2I2,A1)) )
      WRITE(3,476)I,I
  476 FORMAT(6X,2HZ(,I2,1H,,I2,9H)=CTM*SUM)
      WRITE(3,478)I,I
  478 FORMAT(6X,2HDZ,I2,1HS,I2,18H=DCTM*SUM+CTM*DSUM )
      GO TO 490
  475 IF(IS.LT.NSPC)GO TO 480
      WRITE(3,1176)IS,IS,IS,((LBPL,LBCT,KS,LBXSD,KS,IS),KS=1,NM)
      WRITE(3,1180)IS,IS,IS,IS,((LBPL,LBCT,KS,LBDXSD,KS,IS,LBPL,LBDCT,
     * KS,LBXSD,KS,IS),KS=1,NM)
      WRITE(3,476)I,I
      WRITE(3,478)I,I
      GO TO 490
  480 IM=IS-1
      IP=IS+1
      WRITE(3,1176)IS,IS,IS,((LBPL,LBCT,KS,LBXSD,KS,IS),KS=1,IM),
     * ((LBPL,LBCT,KS,LBXSD,IS,KS),KS=IP,NSPC)
      WRITE(3,1180)IS,IS,IS,IS,((LBPL,LBCT,KS,LBDXSD,KS,IS,LBPL,LBDCT,
     * KS,LBXSD,KS,IS),KS=1,IM),((LBPL,LBCT,KS,LBDXSD,IS,KS,LBPL,LBDCT,
     * KS,LBXSD,IS,KS),KS=IP,NSPC)
      WRITE(3,476)I,I
      WRITE(3,478)I,I
  490 CONTINUE
C   SOLVE FOR DIFF VELOCITIES AND ENERGY FLUX.
      WRITE(3,498)
  498 FORMAT(1HC,2X,47HSOLVE FOR DIFFUSION VELOCITIES AND ENERGY FLUX. )
      NMT=LD(NSPC)+2*NSPC
      NDIM=30
      WRITE(3,500)NMT,NDIM
```

```
  500   FORMAT(6X,9HCALL DEC(,I2,1H,,I2,11H,Z,IPS,IER) )                MAIN     800
        DO 495 K=1,NSPC                                                  MAIN     801
        WRITE(3,492)K,K,PHN                                              MAIN     802
  492   FORMAT(6X,2HV(,I2,7H)=RH*DX,I2,1H/,1PE14.6)                      MAIN     803
        WRITE(3,702)K,K,K,PHN                                            MAIN     804
  702   FORMAT(6X,2HDV,I2,8H=(DRH*DX,I2,7H+RH*DDX,I2,2H)/,1PE14.6)       MAIN     805
  495   CONTINUE                                                         MAIN     806
        DO 515 I=1,NSPC                                                  MAIN     807
        IP=I+NSPC                                                        MAIN     808
        WRITE(3,512)IP                                                   MAIN     809
  512   FORMAT(6X,2HV(,I2,5H)=0.0)                                       MAIN     810
        WRITE(3,712)IP                                                   MAIN     811
  712   FORMAT(6X,2HDV,I2,4H=0.0)                                        MAIN     812
  515   CONTINUE                                                         MAIN     813
        DO 517 I=1,NSPC                                                  MAIN     814
        IF(DF(I).EQ.0.0)GO TO 517                                        MAIN     815
        IP=LD(I)+2*NSPC                                                  MAIN     816
        WRITE(3,512)IP                                                   MAIN     817
        WRITE(3,712)IP                                                   MAIN     818
  517   CONTINUE                                                         MAIN     819
        WRITE(3,520)NMT,NDIM                                             MAIN     820
  520   FORMAT(6X,9HCALL SOL(,I2,1H,,I2,9H,Z,V,IPS) )                    MAIN     821
        CALL DR(NSPC,NMT,NDIM)                                           MAIN     822
        DO 525 I=1,NSPC                                                  MAIN     823
        WRITE(3,522)I,I                                                  MAIN     824
  522   FORMAT(6X,2HVX,I2,3H=V(,I2,1H) )                                 MAIN     825
        WRITE(3,722)I,I                                                  MAIN     826
  722   FORMAT(6X,3HDVX,I2,4H=DV(,I2,1H) )                               MAIN     827
  525   CONTINUE                                                         MAIN     828
        DO 528 I=1,NSPC                                                  MAIN     829
        WRITE(3,512)I                                                    MAIN     830
        WRITE(3,712)I                                                    MAIN     831
  528   CONTINUE                                                         MAIN     832
        DO 530 I=1,NSPC                                                  MAIN     833
        IP=I+NSPC                                                        MAIN     834
        WRITE(3,532)IP,I                                                 MAIN     835
        WRITE(3,714)IP,I                                                 MAIN     836
  714   FORMAT(6X,2HDV,I2,3H=DX,I2)                                      MAIN     837
  530   CONTINUE                                                         MAIN     838
  532   FORMAT(6X,2HV(,I2,3H)=X,I2)                                      MAIN     839
        DO 535 I=1,NSPC                                                  MAIN     840
        IF(DF(I).EQ.0.0)GO TO 535                                        MAIN     841
        IP=LD(I)+2*NSPC                                                  MAIN     842
        WRITE(3,532)IP,I                                                 MAIN     843
        WRITE(3,714)IP,I                                                 MAIN     844
  535   CONTINUE                                                         MAIN     845
        WRITE(3,520)NMT,NDIM                                             MAIN     846
        CALL DR(NSPC,NMT,NDIM)                                           MAIN     847
        LBV=2HV(                                                         MAIN     848
        LBP=1H)                                                          MAIN     849
        DO 540 I=1,NSPC                                                  MAIN     850
        WRITE(3,538)I,I,PHN                                              MAIN     851
  538   FORMAT(6X,2HVT,I2,14H=-2.5*RH*DT*V(,I2, 5H)/(T*,1PE14.6,1H) )    MAIN     852
  540   CONTINUE                                                         MAIN     853
        WRITE(3,726)TPN                                                  MAIN     854
  726   FORMAT(6X,15HDDT=UPH2(NPDE)*,1PE14.6)                            MAIN     855
        DO 730 K=1,NSPC                                                  MAIN     856
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```
      WRITE(3,728)K,K,K,K,K,PHN
728   FORMAT(6X,3HDVT,I2,16H=-2.5*(DRH*DT*V(,I2,
     * 11H)+RH*DDT*V(,I2,11H)+RH*DT*DV(,I2,10H)-RH*DT*V(,I2,2H)*,
     * /5X,1H*,1X,9HDT/T)/(T*,1PE14.6,1H) )
730   CONTINUE
      DO 545 I=1,NSPC
      WRITE(3,542)I,I,I,I
542   FORMAT(6X,2HUV,I2,2H=U,I2,4H*(VX,I2,3H+VT,I2,1H) )
545   CONTINUE
      DO 745 I=1,NSPC
      WRITE(3,742)I,I,I,I,I,I,I
742   FORMAT(6X,3HDUV,I2,3H=DU,I2,4H*(VX,I2,3H+VT,I2,1H),
     * 2H+U,I2,5H*(DVX,I2,4H+DVT,I2,1H) )
745   CONTINUE
      DO 550 I=1,NSPC
      WRITE(3,548)I,I
548   FORMAT(6X,9HRHUV(IST+,I2,7H)=RH*UV,I2)
550   CONTINUE
      DO 750 I=1,NSPC
      WRITE(3,748)I,I,I
748   FORMAT(6X,10HDRHUV(IST+,I2,8H)=DRH*UV,I2,7H+RH*DUV,I2)
750   CONTINUE
C  CONVERT FROM CM**3-ATM/SEC-CM-K TO CAL/SEC-CM-K.
      A=-25.0*PRESS*1.9872/(4.0*82.05)
      LBX=1HX
      LBV=3H*V(
      LBTRS=5HRLTRS
      WRITE(3,556)((LBPL,LBX,K,LBV,K+NSPC,LBP),K=1,NSPC)
556   FORMAT(6X,4HSUM=,5(2A1,I2,A3,I2,A1),A1,3(/5X,1H*,1X,
     * 5(A1,I2,A3,I2,2A1)) )
      LBDX=2HDX
      LBDV=4H*DV(
      WRITE(3,756)((LBPL,LBDX,K,LBV,K+NSPC,LBP,LBPL,LBX,K,LBDV,
     * K+NSPC,LBP),K=1,NSPC)
756   FORMAT(6X,5HDSUM=,2(A1,A2,I2,A3,I2,3A1,I2,A4,I2,A1),A1,
     * 6(/5X,1H*,3(A2,I2,A3,I2,3A1,I2,A4,I2,2A1)) )
      WRITE(3,557)LBTRS,A
557   FORMAT(6X,A5,1H=,1PE14.6,6H*SUM/T)
      LBDTRS=6HDRLTRS
      WRITE(3,757)LBDTRS,A
757   FORMAT(6X,A6,1H=,1PE14.6,18H*(DSUM-SUM*DT/T)/T )
      LBINT=5HRLINT
      DO 553 I=1,NSPC
      IF(DF(I).EQ.0.0)GO TO 553
      J=LD(I)
      LDV(J)=I
553   CONTINUE
      NT=LD(NSPC)
      IF(NT.EQ.0)GO TO 554
      WRITE(3,556)((LBPL,LBX,LDV(K),LBV,K+2*NSPC,LBP),K=1,NT)
      WRITE(3,756)((LBPL,LBDX,LDV(K),LBV,K+2*NSPC,LBP,LBPL,LBX,LDV(K),
     * LBDV,K+2*NSPC,LBP),K=1,NT)
      WRITE(3,557)LBINT,A
      LBDINT=6HDRLINT
      WRITE(3,757)LBDINT,A
554   CONTINUE
      WRITE(3,562)
```

```
 562  FORMAT(6X,15HRLM=RLTRS+RLINT )
      WRITE(3,762)
 762  FORMAT(6X,18HDRLM=DRLTRS+DRLINT)
      WRITE(3,566)
 566  FORMAT(6X,15HRHLM(IC)=RH*RLM)
      WRITE(3,766)
 766  FORMAT(6X,25HDRHLM(IC)=DRH*RLM+RH*DRLM )
      LBDX=2HDX
      WRITE(3,570)((LBPL,LBDX,L,LBV,L,LBP),L=1,NSPC)
 570  FORMAT(6X,4HSUM=,5(A1,A2,I2,A3,I2,A1),A1,3(/5X,1H*,1X,
     * 5(A2,I2,A3,I2,2A1)) )
      LBDDX=3HDDX
      WRITE(3,770)((LBPL,LBDDX,L,LBV,L,LBP,LBPL,LBDX,L,LBDV,L,LBP),
     * L=1,NSPC)
 770  FORMAT(6X,5HDSUM=,2(A1,A3,I2,A3,I2,2A1,A2,I2,A4,I2,A1),A1,
     * 9(/5X,1H*,1X,2(A3,I2,A3,I2,2A1,A2,I2,A4,I2,2A1)) )
      A=-2.5*1.9872*PRESS/(82.05*PHN)
      WRITE(3,572)A
 572  FORMAT(6X,3HQX=,1PE20.12,7H*RH*SUM)
      WRITE(3,772)A
 772  FORMAT(6X,8HDQX(IC)=,1PE20.12,18H*(DRH*SUM+RH*DSUM))
C  ************************
C  FIND THE TIME DERIVATIVES.
C  ************************
      WRITE(3,612)
 612  FORMAT(1HC,2X,26HFIND THE TIME DERIVATIVES.)
      WRITE(3,622)
 622  FORMAT(6X,15HSP=ASP+BSP*TIME)
      TMSPH2=TMN/(PHN*PHN)
      WRITE(3,628)
 628  FORMAT(1X,3H100,2X,8HCONTINUE)
      WRITE(3,632)
 632  FORMAT(6X,25HIF(KPDE.EQ.NPDE)GO TO 150)
      WRITE(3,636)TMN
 636  FORMAT(6X,3HRY=,1PE20.10,8H*R(KPDE) )
      TMSPH=TMN/PHN
      WRITE(3,638)TMSPH
 638  FORMAT(6X,4HDY=-,1PE20.10,16H*DRHUV(IST+KPDE)   )
      WRITE(3,642)
 642  FORMAT(6X,23HFVAL=SP*UPH(KPDE)+DY+RY)
      WRITE(3,646)
 646  FORMAT(6X,6HRETURN)
      WRITE(3,648)
 648  FORMAT(1X,3H150,2X,8HCONTINUE)
      WRITE(3,662)TMSPH2
 662  FORMAT(6X,3HTL=,1PE20.10,1H*)
      WRITE(3,664)
 664  FORMAT(5X,1H*,1X,41H(DRHLM(IC)*UPH(NPDE)+RHLM(IC)*UPH2(NPDE)) )
      LBBL=1H
      LBC=6HC(IST+
      LBRHUV=10H)*RHUV(IST
      WRITE(3,668)TMSPH,((LBBL,LBPL,LBC,K,LBRHUV,LBPL,K,LBP),K=1,NSPC)
     * ,LBP
 668  FORMAT(6X,4HTD=-,1PE20.10,12H*UPH(NPDE)*(,2A1,A6,I2,A10,A1,I2,3A1,
     * 10(/5X,1H*,1X,2(A6,I2,A10,A1,I2,3A1)) )
      TMSTP=TMN/TPN
      LBR=2HR(
```

```
      LBH=8H)*H(IST+
      WRITE(3,672)TMSTP,((LBBL,LBPL,LHR,K,LBH,K,LBP),K=1,NSPC),LBP
  672 FORMAT(6X,4HTR=-,1PE20.10,2H*(,2(2A1,A2,I2,A8,I2,A1),2A1,
     * 9(/5X,1H*,1X,2(A2,I2,A8,I2,3A1)) )
      A=-TMN/(TPN*PHN)
      WRITE(3,674)A
  674 FORMAT(6X,3HTX=,1PE20.I2,8H*DQX(IC) )
      WRITE(3,676)
  676 FORMAT(6X,38HFVAL=SP*UPH(NPDE)+(TL+TR+TD+TX)/CM(IC) )
      STOP
      END
```

```
      SUBROUTINE DR(NSPC,NMT,NDIM)
C  FIND THE DERIVATIVES OF THE SOLUTIONS V.
      LBDZ=2HDZ
      LBSP=1HS
      LBM=1H-
      LBV=3H*V(
      LBP=1H)
      I=1
      NTOP=2*NSPC
      WRITE(3,10)I,I,((LBM,LBDZ,I,LBSP,J,LBV,J,LBP),J=2,NTOP)
   10 FORMAT(6X,3HDV(,I2,4H)=DV,I2,3(A1,A2,I2,A1,I2,A3,I2,A1),A1,
     * 7(/5X,1H*,1X,4(A2,I2,A1,I2,A3,I2,2A1)) )
      NM=NSPC-1
      DO 15 I=2,NM
      IM=I-1
      IP=I+1
      NST=NSPC+1
      WRITE(3,10)I,I,((LBM,LBDZ,I,LBSP,J,LBV,J,LBP),J=1,IM),
     * ((LBM,LBDZ,I,LBSP,J,LBV,J,LBP),J=IP,NSPC),
     * ((LBM,LBDZ,I,LBSP,J,LBV,J,LBP),J=NST,NTOP)
   15 CONTINUE
      I=NSPC
      WRITE(3,10)I,I,((LBM,LBDZ,I,LBSP,J,LBV,J,LBP),J=1,NM),
     * ((LBM,LBDZ,I,LBSP,J,LBV,J,LBP),J=NST,NTOP)
      DO 25 I=1,NSPC
      IP=I+NSPC
      WRITE(3,10)IP,IP,((LBM,LBDZ,IP,LBSP,J,LBV,J,LBP),J=1,NMT)
   25 CONTINUE
      ITOP=NMT-2.0*NSPC
      DO 30 I=1,ITOP
      IP=I+2*NSPC
      WRITE(3,10)IP,IP,((LBM,LBDZ,IP,LBSP,J,LBV,J,LBP),J=NST,NTOP),
     * LBM,LBDZ,IP,LBSP,IP,LBV,IP,LBP
   30 CONTINUE
      WRITE(3,32)NMT,NDIM
   32 FORMAT(6X,9HCALL SOL(,I2,1H,,I2,10H,Z,DV,IPS) )
      RETURN
      END
```

```
        S C O P E   2   L O A D   M A P                              LOADER VERSION 1.0   04/15/80  14.18.13.  PAGE    1
PROGRAM WILL BE ENTERED AT  LOADF      (   241)                      SCM LENGTH     25140          LCM LENGTH          0

        BLOCK           ADDRESS     LENGTH      FILE

        LOADF             110       17367       LGO
        DR              17477         401       LGO
         /STP.END/      20100           1     SL-FTNLIB
         /FCL.C./       20101          30     SL-FTNLIB
         /Q8.IO./       20131         144     SL-FTNLIB
        Q2NTRY=         20275           4     SL-FTNLIB
        COMIO=          20301          10     SL-FTNLIB
        FECMSK=         20311          41     SL-FTNLIB
        FEIFST=         20352           3     SL-FTNLIB
        FLTIN=          20355         156     SL-FTNLIB
        FLTOUT=         20533         315     SL-FTNLIB
        FMTAP=          21050         377     SL-FTNLIB
        FORSYS=         21447         300     SL-FTNLIB
        FORUTL=         21747          45     SL-FTNLIB
        GETFIT=         22014          54     SL-FTNLIB
        INCOM=          22070         144     SL-FTNLIB
        INPC=           22234         173     SL-FTNLIB
        KODER=          22427         476     SL-FTNLIB
        KRAKER=         23125         454     SL-FTNLIB
        OUTC=           23601         155     SL-FTNLIB
        OUTCOM=         23756         204     SL-FTNLIB
        SPA=            24162          11     SL-FTNLIB
        ERRCAP=         24173         317     SL-FTNLIB
        FERCAP=         24512         171     SL-FTNLIB
        ACOS            24703           6     SL-FTNLIB
        ACOSIN.         24711          63     SL-FTNLIB
        EXP.MSG         24774          16     SL-FTNLIB
        SQRT            25012           6     SL-FTNLIB
        SQRT.           25020          32     SL-FTNLIB
        SYSAID=         25052           1     SL-FTNLIB
        SYS=1ST         25053          65     SL-FTNLIB

   1    H2            2.00     2.00     2.92    38.00      0.00      .79   280.00      CNST

 .31001901E+01  .51119464E-03  .52644210E-07 -.34909973E-10  .36945345E-14   H2
-.87738042E+03 -.19629421E+01  .30574451E+01  .26765200E-02 -.58099162E-05   H2
 .55210391E-08 -.18122739E-11 -.98890474E+03 -.22997056E+01                  H2

   2    N2           28.00     2.00     3.62    97.50      0.00     0.00    15.70       VAR

 .28963194E+01  .15154866E-02 -.57235277E-06  .99807393E-10 -.65223555E-14   N2
-.90586184E+03  .61615148E+01  .36748261E+01 -.12081500E-02  .23240102E-05   N2
-.63217559E-09 -.22577253E-12 -.10611588E+04  .23580424E+01                  N2

   1    H2        2.188700E-06  6.502900E-01     H2      VISCOSITY.

   1    H2        6.357900E-06  7.383300E-01     H2      THERMAL CONDUCTIVITY.

   2    N2        4.266700E-06  6.613600E-01     N2      VISCOSITY.

   2    N2        6.407700E-07  7.999600E-01     N2      THERMAL CONDUCTIVITY.
```

```
 1       1    H2      H2        1.119300E-04  1.661400E+00    H2        H2     BINARY DIFFUSION.

 1       2    H2      N2        5.951700E-05  1.663800E+00    H2        N2     BINARY DIFFUSION.

 2       2    N2      N2        1.537400E-05  1.672900E+00    N2        N2     BINARY DIFFUSION.
PRESS =  1.00
TPN =  1.0000E+03      PHN =  5.0000E-05      TMN =  1.0000E-03

 1.088500E+00  9.055700E-03   A*  HCB   FIT A*TS**B

 1.078600E+00  8.500100E-02   B*  HCB  FIT  A*EXP(C/T)

 9.542600E-01 -1.435700E-01   C*  HCB  FIT  A*EXP(C/T)
```

```
      SUBROUTINE F(TIME,PH,U,UPH,UPH2,FVAL,NPDE,KPDE,IC,KSKT,KSKR)
      DIMENSION Z(30,30),IPS(30)
      DIMENSION V(30),DV(30)
      DIMENSION U(NPDE),UPH(NPDE),UPH2(NPDE)
      COMMON/TABAB/ASP,BSP,TPN,PHN,TMN,TMSPH,TMSPH2,TMSTP,TPENT
      COMMON/TABP/PRESS,PSR,NPDEM
      COMMON/TABSM/SMALL
      COMMON/TABAM/YAB,WAB
      DIMENSION R(20)
      DIMENSION C(1000),H(1000),RHLM(100),DRHLM(100),CM(100)
      DIMENSION DC(1000)
      DIMENSION DQX(100)
      COMMON/TABCT/RL,CPMX,HO(20),R2D(20),R2DM(20)
      COMMON/TABMF/RHUV(1000),DRHUV(1000)
      COMMON/TABRY/T,RH,Y1,Y2,Y3,Y4,Y5,Y6,Y7,Y8,Y9,Y10
C  AT EACH CALL THE TIME RATE OF CHANGE FOR ONE PDE IS RETURNED IN FVAL.
C  WE WANT TO AVOID DIVISION BY ZERO.
      DO 5 K=1,NPDEM
      IF(ABS(U(K)).LT.SMALL)U(K)=SMALL
    5 IF(ABS(UPH(K)).LT.SMALL)UPH(K)=SMALL
C  TEST CASE.  BINARY MIX OF H2 AND N2.  TRANSPORT WARNATZ PAR.
C  U = MASS FRACTIONS.  Y = MASS FRACTIONS / MOLECULAR WEIGHTS.
      YN=1.0-U( 1)
      CALL RT(U,YN,R,NPDE,KPDE,IC,KSKR)
      IST= 2*(IC-1)
      DT=UPH(NPDE)*  1.000000E+03
      IF(KSKT.GT.1)GO TO 100
      IF(KSKR.GT.1)GO TO 125
C  NTIS ENTHALPIES AND HEAT CAPACITIES.
      IF(T.GT.1000.)GO TO 2000
      C 1=1.9872*(  3.05744510E+00+T*(  2.67652000E-03
     * +T*( -5.80991620E-06+T*(  5.52103910E-09+T*( -1.81227390E-12)))))
      DC 1=1.9872*(  2.67652000E-03+T*( -1.16198324E-05
     * +T*(  1.65631173E-08+T*( -7.24909560E-12))))*DT
      H 1=1.9872*( -9.88904740E+02+T*(  3.05744510E+00
     * +T*(  2.67652000E-03/2.0+T*( -5.80991620E-06/3.0
     * +T*(  5.52103910E-09/4.0+T*( -1.81227390E-12/5.0))))))
      C 2=1.9872*(  3.67482610E+00+T*( -1.20815000E-03
     * +T*(  2.32401020E-06+T*( -6.32175590E-10+T*( -2.25772530E-13)))))
      DC 2=1.9872*( -1.20815000E-03+T*(  4.64802040E-06
     * +T*( -1.89652677E-09+T*( -9.03090120E-13))))*DT
      H 2=1.9872*( -1.06115880E+03+T*(  3.67482610E+00
     * +T*( -1.20815000E-03/2.0+T*(  2.32401020E-06/3.0
     * +T*( -6.32175590E-10/4.0+T*( -2.25772530E-13/5.0))))))
      GO TO 3000
 2000 CONTINUE
      C 1=1.9872*(  3.10019010E+00+T*(  5.11194640E-04
     * +T*(  5.26442100E-08+T*( -3.49099730E-11+T*(  3.69453450E-15)))))
      DC 1=1.9872*(  5.11194640E-04+T*(  1.05288420E-07
     * +T*( -1.04729919E-10+T*(  1.47781380E-14))))*DT
      H 1=1.9872*( -8.77380420E+02+T*(  3.10019010E+00
     * +T*(  5.11194640E-04/2.0+T*(  5.26442100E-08/3.0
     * +T*( -3.49099730E-11/4.0+T*(  3.69453450E-15/5.0))))))
      C 2=1.9872*(  2.89631940E+00+T*(  1.51548660E-03
     * +T*( -5.72352770E-07+T*(  9.98073930E-11+T*( -6.52235550E-15)))))
      DC 2=1.9872*(  1.51548660E-03+T*( -1.14470554E-06
     * +T*(  2.99422179E-10+T*( -2.60894220E-14))))*DT
```

```
      H 2=1.9872*( -9.05861840E+02+T*(  2.89631940E+00
     * +T*(  1.51548660E-03/2.0+T*( -5.72352770E-07/3.0
     * +T*(  9.98073930E-11/4.0+T*( -6.52235550E-15/5.0))))))
 3000 CONTINUE
C  SPECIFIC HEATS AND SPECIFIC ENTHALPIES.
      C(IST+ 1)=C 1/  2.00
      DC(IST+ 1)=DC 1/  2.00
      H(IST+ 1)=H 1/  2.00
      C(IST+ 2)=C 2/ 28.00
      DC(IST+ 2)=DC 2/ 28.00
      H(IST+ 2)=H 2/ 28.00
  125 CONTINUE
C  VISCOSITY FROM WARNATZ ST PAR.
C  LEAST SQUARES FIT,  T=300,2000.
C  THERMAL CONDUCTIVITIES FROM WARNATZ ST PAR.
C  LEAST SQUARES FIT,  T=300,2000.
C     V 1=  2.188700E-06*(T**  6.502900E-01)
C     V 2=  4.266700E-06*(T**  6.613600E-01)
C     RL 1=  6.357900E-06*(T**  7.383300E-01)
C     RL 2=  6.407700E-07*(T**  7.999600E-01)
C  BINARY DIFFUSION COEFFICIENTS FROM WARNATZ ST PAR.
C  LEAST SQUARES FIT,  T=300,2000.
C  PRESS =  1.00
C     D 1 1=  1.119300E-04*(T**  1.661400E+00)
C     D 1 2=  5.951700E-05*(T**  1.663800E+00)
C     D 2 2=  1.537400E-05*(T**  1.672900E+00)
C  DEFINE USEFUL COMBINATIONS AND DERIVATIVES
      YS=Y 3
      X 1=Y 1/YS
      X 2=Y 2/YS
      U 1=U( 1)
      DU 1=UPH( 1)
      DDU 1=UPH2( 1)
      U 2=1.0-U 1
      DU 2=-DU 1
      DDU 2=-DDU 1
      DY 1=DU 1/  2.00
      DY 2=DU 2/ 28.00
      DYS=+DY 1+DY 2
      DDY 1=DDU 1/  2.00
      DDY 2=DDU 2/ 28.00
      DDYS=+DDY 1+DDY 2
C  TPN =  1.0000E+03      PHN =  5.0000E-05      TMN =  1.0000E-03
      DRH=-  1.218769043266E-02*(DT/T+DYS/YS)/(T*YS)
      DYSY=DYS/(YS*YS)
      DYSYSQ=(DYS/YS)**2
      DX 1=DY 1/YS-Y 1*DYSY
      DDX 1=(DDY 1-2.0*DY 1*DYS/YS+2.0*Y 1*DYSYSQ-Y 1*DDYS/YS)/YS
      CSZR 1=  3.571428571429E-03
      DCSZR 1=0.0
      CZ 1 1=1.0+  1.061032953946E+00*(CSZR 1)
      DCZ 1 1=  1.061032953946E+00*(DCSZR 1)
      CINT 1=C(IST+ 1)*  1.006441223833E+00-2.5
      DCINT 1=DC(IST+ 1)*  1.006441223833E+00
      CSC 1=CSZR 1/CINT 1
      DCSC 1=(DCSZR 1-CSZR 1*DCINT 1/CINT 1)/CINT 1
      DX 2=DY 2/YS-Y 2*DYSY
```

```
      DDX 2=(DDY 2-2.0*DY 2*DYS/YS+2.0*Y 2*DYSYSQ-Y 2*DDYS/YS)/YS
      CSZR 2=  6.369426751592E-02+  1.751045651893E+00/
     * SQRT(T)+  3.483292299373E+01/T
      DCSZR 2=-( 8.755228259466E-01/SQRT(T)+ 3.483292299373E+01/T)*DT/T
      CZ 2 2=1.0+  1.061032953946E+00*(CSZR 2)
      DCZ 2 2=  1.061032953946E+00*(DCSZR 2)
      CINT 2=C(1ST+ 2)*  1.409017713366E+01-2.5
      DCINT 2=DC(1ST+ 2)*  1.409017713366E+01
      CSC 2=CSZR 2/CINT 2
      DCSC 2=(DCSZR 2-CSZR 2*DCINT 2/CINT 2)/CINT 2
      X 1 1=X 1*X 1
      DX 1 1=DX 1*X 1+X 1*DX 1
      VD 1 1=  8.934155275619E+03*(T**( -1.661400E+00))
      DVD 1 1= -1.484320557491E+04*(T**( -2.661400E+00))*DT
      XSD 1 1=X 1 1*VD 1 1
      DXSD 1 1=DX 1 1*VD 1 1+X 1 1*DVD 1 1
      X 1 2=X 1*X 2
      DX 1 2=DX 1*X 2+X 1*DX 2
      VD 1 2=  1.680192213989E+04*(T**( -1.663800E+00))
      DVD 1 2= -2.795503805635E+04*(T**( -2.663800E+00))*DT
      XSD 1 2=X 1 2*VD 1 2
      DXSD 1 2=DX 1 2*VD 1 2+X 1 2*DVD 1 2
      CZ 1 2=1.0+  5.305164769730E-01*(CSZR 1+CSZR 2)
      DCZ 1 2=  5.305164769730E-01*(DCSZR 1+DCSZR 2)
      X 2 2=X 2*X 2
      DX 2 2=DX 2*X 2+X 2*DX 2
      VD 2 2=  6.504488096787E+04*(T**( -1.672900E+00))
      DVD 2 2= -1.088135813711E+05*(T**( -2.672900E+00))*DT
      XSD 2 2=X 2 2*VD 2 2
      DXSD 2 2=DX 2 2*VD 2 2+X 2 2*DVD 2 2
      SXSD 1=+X 2*VD 1 2
      DSXSD 1=+DX 2*VD 1 2+X 2*DVD 1 2
      SXSD 2=+X 1*VD 1 2+X 3*VD 2 3
      DSXSD 2=+DX 1*VD 1 2+X 1*DVD 1 2+DX 3*VD 2 3+X 3*DVD 2 3
      SXSD 2=+X 1*VD 1 2
      DSXSD 2=+DX 1*VD 1 2+X 1*DVD 1 2
      STV 1=  4.568922191255E+05*(T**( -1.650290E+00))
      DSTV 1= -7.540046603006E+05*(T**( -2.650290E+00))*DT
      XSTV 1=X 1 1*STV 1
      DXSTV 1=DX 1 1*STV 1+X 1 1*DSTV 1
      STV 2=  2.343731689596E+05*(T**( -1.661360E+00))
      DSTV 2= -3.893782079828E+05*(T**( -2.661360E+00))*DT
      XSTV 2=X 2 2*STV 2
      DXSTV 2=DX 2 2*STV 2+X 2 2*DSTV 2
C  SPECIFIC HEAT OF THE MIXTURE.  NTIS FORMULA.
      CM(IC)=+C(1ST+ 1)*U 1+C(1ST+ 2)*U 2
C  DIFFUSION AND HEAT FLUX.
C  SEE DIXON-LEWIS.
C  11.  TRANSPORT PHENOMENA IN MULTICOMPONENT SYSTEMS.
C  LM 00.00
      Z( 1, 1)=0.0
      Z( 2, 2)=0.0
      Z( 1, 2)=XSD 1 2+  1.400000000000E+01*X 2*SXSD 1
      DZ 1S 2=DXSD 1 2+  1.400000000000E+01*(DX 2*SXSD 1+X 2*DSXSD 1)
      Z( 2, 1)=XSD 1 2+  7.142857142857E-02*X 1*SXSD 2
      DZ 2S 1=DXSD 1 2+  7.142857142857E-02*(DX 1*SXSD 2+X 1*DSXSD 2)
C  FIND T*, A*, B*, AND C*.
```

```
      TS=T/  6.086871E+01
      DTS=DT/  6.086871E+01
      AST 1 2=  1.088500E+00*(TS**(  9.055700E-03))
      DAST 1 2=  9.857129450000E-03*DTS*(TS**( -9.909443E-01))
      EX=EXP(  8.500100E-02/TS)
      BST 1 2=  1.078600E+00*EX
      DBST 1 2= -9.168208E-02*DTS*EX/(TS*TS)
      EX=EXP( -1.435700E-01/TS)
      CST 1 2=  9.542600E-01*EX
      DCST 1 2=  1.370031E-01*DTS*EX/(TS*TS)
C  LM 00,10 AND LM 10,00
      CT= -1.666666666667E-01*(1.2*CST 1 2-1.0)
      DCT= -2.000000000000E-01*DCST 1 2
      Z( 1, 4)=CT*XSD 1 2
      DZ 1S 4=CT*DXSD 1 2+DCT*XSD 1 2
      CT= -2.333333333333E+00*(1.2*CST 1 2-1.0)
      DCT= -2.800000000000E+00*DCST 1 2
      Z( 2, 3)=CT*XSD 1 2
      DZ 2S 3=CT*DXSD 1 2+DCT*XSD 1 2
      Z( 1, 3)=-Z( 2, 3)
      DZ 1S 3=-DZ 2S 3
      Z( 2, 4)=-Z( 1, 4)-Z( 3, 4)
      DZ 2S 4=-DZ 1S 4-DZ 3S 4
      Z( 2, 4)=-Z( 1, 4)
      DZ 2S 4=-DZ 1S 4
      Z( 3, 1)=Z( 1, 3)
      DZ 3S 1=DZ 1S 3
      Z( 3, 2)=Z( 2, 3)
      DZ 3S 2=DZ 2S 3
      Z( 4, 1)=Z( 1, 4)
      DZ 4S 1=DZ 1S 4
      Z( 4, 2)=Z( 2, 4)
      DZ 4S 2=DZ 2S 4
C  LM 01,00 AND LM 00,01
      Z( 5, 1)=0.0
      Z( 5, 2)=0.0
      Z( 6, 1)=0.0
      Z( 6, 2)=0.0
      Z( 1, 5)=0.0
      Z( 1, 6)=0.0
      Z( 2, 5)=0.0
      Z( 2, 6)=0.0
C  LM 10,10
      CT=  6.222222222222E-02*(13.75-3.0*BST 1 2-4.0*AST 1 2*CZ 1 2)
      DCT=-  6.222222222222E-02*(3.0*DBST 1 2+4.0*(AST 1 2*DCZ 1 2
     * +DAST 1 2*CZ 1 2))
      Z( 3, 4)=CT*XSD 1 2
      Z( 4, 3)=Z( 3, 4)
      DZ 3S 4=CT*DXSD 1 2+DCT*XSD 1 2
      DZ 4S 3=DZ 3S 4
      CT= -4.062563477554E-02*CZ 1 1
      DCT= -4.062563477554E-02*DCZ 1 1
      CT 2=  2.488888888889E-01*AST 1 2*CZ 1 2
      DCT 2=  2.488888888889E-01*(DAST 1 2*CZ 1 2+AST 1 2*DCZ 1 2)
      CT 2=  5.477777777778E+00-  2.613333333333E+00*BST 1 2+CT 2
      DCT 2=-  2.613333333333E+00*DBST 1 2+DCT 2
      Z( 3, 3)=CT*XSTV 1-XSD 1 2*CT 2
```

```
      DZ 3S 3=CT*DXSTV 1+DCT*XSTV 1-DXSD 1 2*CT 2-XSD 1 2*DCT 2
      CT= -5.687588868576E-01*CZ 2 2
      DCT= -5.687588868576E-01*DCZ 2 2
      CT 1=  2.488888888889E-01*AST 1 2*CZ 1 2
      DCT 1=  2.488888888889E-01*(DAST 1 2*CZ 1 2+AST 1 2*DCZ 1 2)
      CT 1=  6.561111111111E+00-  1.333333333333E-02*BST 1 2+CT 1
      DCT 1=-  1.333333333333E-02*DBST 1 2+DCT 1
      Z( 4, 4)=CT*XSTV 2-XSD 1 2*CT 1
      DZ 4S 4=CT*DXSTV 2+DCT*XSTV 2-DXSD 1 2*CT 1-XSD 1 2*DCT 1
C  LM 10,01 AND LM 01,10
      CT=  2.970892271049E+00*AST 1 2*CSC 2
      DCT=  2.970892271049E+00*(DAST 1 2*CSC 2+AST 1 2*DCSC 2)
      Z( 3, 6)=XSD 1 2*CT
      DZ 3S 6=DXSD 1 2*CT+XSD 1 2*DCT
      CT=  2.122065907892E-01*AST 1 2*CSC 1
      DCT=  2.122065907892E-01*(DAST 1 2*CSC 1+AST 1 2*DCSC 1)
      Z( 4, 5)=XSD 1 2*CT
      DZ 4S 5=DXSD 1 2*CT+XSD 1 2*DCT
      CT=  6.465770590774E-02*CSC 1
      DCT=  6.465770590774E-02*DCSC 1
      CT 2=  2.122065907892E-01*AST 1 2*CSC 1
      DCT 2=  2.122065907892E-01*(DAST 1 2*CSC 1+AST 1 2*DCSC 1)
      Z( 3, 5)=CT*XSTV 1+CT 2*XSD 1 2
      DZ 3S 5=CT*DXSTV 1+DCT*XSTV 1+CT 2*DXSD 1 2+DCT 2*XSD 1 2
      CT=  9.052078827083E-01*CSC 2
      DCT=  9.052078827083E-01*DCSC 2
      CT 1=  2.970892271049E+00*AST 1 2*CSC 2
      DCT 1=  2.970892271049E+00*(DAST 1 2*CSC 2+AST 1 2*DCSC 2)
      Z( 4, 6)=CT*XSTV 2+CT 1*XSD 1 2
      DZ 4S 6=CT*DXSTV 2+DCT*XSTV 2+CT 1*DXSD 1 2+DCT 1*XSD 1 2
      Z( 5, 3)=Z( 3, 5)
      DZ 5S 3=DZ 3S 5
      Z( 5, 4)=Z( 4, 5)
      DZ 5S 4=DZ 4S 5
      Z( 6, 3)=Z( 3, 6)
      DZ 6S 3=DZ 3S 6
      Z( 6, 4)=Z( 4, 6)
      DZ 6S 4=DZ 4S 6
C  LM 01,01
      Z( 5, 6)=0.0
      Z( 6, 5)=0.0
      CTM=-6.25/CINT 1
      DCTM=6.25*DCINT 1/(CINT 1*CINT 1)
      CT=  1.551784941786E-02*CSC 1
      DCT=  1.551784941786E-02*DCSC 1
      CT 2=1.0+  5.456740906008E-02*AST 1 2*CSC 1
      DCT 2=  5.456740906008E-02*(DAST 1 2*CSC 1+AST 1 2*DCSC 1)
      SUM=CT*XSTV 1+XSD 1 1+CT 2*XSD 1 2
      DSUM=DCT*XSTV 1+CT*DXSTV 1+DXSD 1 1+CT 2*DXSD 1 2+DCT 2*XSD 1 2
      Z( 5, 5)=CTM*SUM
      DZ 5S 5=DCTM*SUM+CTM*DSUM
      CTM=-6.25/CINT 2
      DCTM=6.25*DCINT 2/(CINT 2*CINT 2)
      CT=  2.172498918500E-01*CSC 2
      DCT=  2.172498918500E-01*DCSC 2
      CT 1=1.0+  1.069521217578E+01*AST 1 2*CSC 2
      DCT 1=  1.069521217578E+01*(DAST 1 2*CSC 2+AST 1 2*DCSC 2)
```

```
      SUM=CT*XSTV 2+XSD 2 2+CT 1*XSD 1 2
      DSUM=DCT*XSTV 2+CT*DXSTV 2+DXSD 2 2+CT 1*DXSD 1 2+DCT 1*XSD 1 2
      Z( 6, 6)=CTM*SUM
      DZ 65 6=DCTM*SUM+CTM*DSUM
C  SOLVE FOR DIFFUSION VELOCITIES AND ENERGY FLUX.
      CALL DEC( 6,30,Z,1PS,IER)
      V( 1)=RH*DX 1/  5.000000E-05
      DV 1=(DRH*DX 1+RH*DDX 1)/  5.000000E-05
      V( 2)=RH*DX 2/  5.000000E-05
      DV 2=(DRH*DX 2+RH*DDX 2)/  5.000000E-05
      V( 3)=0.0
      DV 3=0.0
      V( 4)=0.0
      DV 4=0.0
      V( 5)=0.0
      DV 5=0.0
      V( 6)=0.0
      DV 6=0.0
      CALL SOL( 6,30,Z,V,1PS)
      DV( 1)=DV 1-DZ 15 2*V( 2)-DZ 15 3*V( 3)-DZ 15 4*V( 4)
      DV( 2)=DV 2-DZ 25 1*V( 1)-DZ 25 3*V( 3)-DZ 25 3*V( 3)-
     * DZ 25 4*V( 4)
      DV( 2)=DV 2-DZ 25 1*V( 1)-DZ 25 3*V( 3)-DZ 25 4*V( 4)
      DV( 3)=DV 3-DZ 35 1*V( 1)-DZ 35 2*V( 2)-DZ 35 3*V( 3)-
     * DZ 35 4*V( 4)-DZ 35 5*V( 5)-DZ 35 6*V( 6)
      DV( 4)=DV 4-DZ 45 1*V( 1)-DZ 45 2*V( 2)-DZ 45 3*V( 3)-
     * DZ 45 4*V( 4)-DZ 45 5*V( 5)-DZ 45 6*V( 6)
      DV( 5)=DV 5-DZ 55 3*V( 3)-DZ 55 4*V( 4)-DZ 55 5*V( 5)
      DV( 6)=DV 6-DZ 65 3*V( 3)-DZ 65 4*V( 4)-DZ 65 6*V( 6)
      CALL SOL( 6,30,Z,DV,1PS)
      VX 1=V( 1)
      DVX 1=DV( 1)
      VX 2=V( 2)
      DVX 2=DV( 2)
      V( 1)=0.0
      DV 1=0.0
      V( 2)=0.0
      DV 2=0.0
      V( 3)=X 1
      DV 3=DX 1
      V( 4)=X 2
      DV 4=DX 2
      V( 5)=X 1
      DV 5=DX 1
      V( 6)=X 2
      DV 6=DX 2
      CALL SOL( 6,30,Z,V,1PS)
      DV( 1)=DV 1-DZ 15 2*V( 2)-DZ 15 3*V( 3)-DZ 15 4*V( 4)
      DV( 2)=DV 2-DZ 25 1*V( 1)-DZ 25 3*V( 3)-DZ 25 3*V( 3)-
     * DZ 25 4*V( 4)
      DV( 2)=DV 2-DZ 25 1*V( 1)-DZ 25 3*V( 3)-DZ 25 4*V( 4)
      DV( 3)=DV 3-DZ 35 1*V( 1)-DZ 35 2*V( 2)-DZ 35 3*V( 3)-
     * DZ 35 4*V( 4)-DZ 35 5*V( 5)-DZ 35 6*V( 6)
      DV( 4)=DV 4-DZ 45 1*V( 1)-DZ 45 2*V( 2)-DZ 45 3*V( 3)-
     * DZ 45 4*V( 4)-DZ 45 5*V( 5)-DZ 45 6*V( 6)
      DV( 5)=DV 5-DZ 55 3*V( 3)-DZ 55 4*V( 4)-DZ 55 5*V( 5)
      DV( 6)=DV 6-DZ 65 3*V( 3)-DZ 65 4*V( 4)-DZ 65 6*V( 6)
```

```
      CALL SDL( 6,30,Z,DV,1PS)
      VT 1=-2.5*RH*DT*V( 1)/(T*  5.000000E-05)
      VT 2=-2.5*RH*DT*V( 2)/(T*  5.000000E-05)
      DDT=UPH2(NPDE)*  1.000000E+03
      DVT 1=-2.5*(DRH*DT*V( 1)+RH*DDT*V( 1)+RH*DT*DV( 1)-RH*DT*V( 1)*
     * DT/T)/(T*  5.000000E-05)
      DVT 2=-2.5*(DRH*DT*V( 2)+RH*DDT*V( 2)+RH*DT*DV( 2)-RH*DT*V( 2)*
     * DT/T)/(T*  5.000000E-05)
      UV 1=U 1*(VX 1+VT 1)
      UV 2=U 2*(VX 2+VT 2)
      DUV 1=DU 1*(VX 1+VT 1)+U 1*(DVX 1+DVT 1)
      DUV 2=DU 2*(VX 2+VT 2)+U 2*(DVX 2+DVT 2)
      RHUV(IST+ 1)=RH*UV 1
      RHUV(IST+ 2)=RH*UV 2
      DRHUV(IST+ 1)=DRH*UV 1+RH*DUV 1
      DRHUV(IST+ 2)=DRH*UV 2+RH*DUV 2
      SUM=+X 1*V( 3)+X 2*V( 4)
      DSUM=+DX 1*V( 3)+X 1*DV( 3)+DX 2*V( 4)+X 2*DV( 4)
      RLTRS= -1.513711E-01*SUM/T
      DRLTRS= -1.513711E-01*(DSUM-SUM*DT/T)/T
      SUM=+X 1*V( 5)+X 2*V( 6)
      DSUM=+DX 1*V( 5)+X 1*DV( 5)+DX 2*V( 6)+X 2*DV( 6)
      RLINT= -1.513711E-01*SUM/T
      DRLINT= -1.513711E-01*(DSUM-SUM*DT/T)/T
      RLM=RLTRS+RLINT
      DRLM=DRLTRS+DRLINT
      RHLM(IC)=RH*RLM
      DRHLM(IC)=DRH*RLM+RH*DRLM
      SUM=+DX 1*V( 1)+DX 2*V( 2)
      DSUM=+DDX 1*V( 1)+DX 1*DV( 1)+DDX 2*V( 2)+DX 2*DV( 2)
      QX= -1.210968921389E+03*RH*SUM
      DQX(IC)= -1.210968921389E+03*(DRH*SUM+RH*DSUM)
C  FIND THE TIME DERIVATIVES.
      SP=ASP+BSP*TIME
  100 CONTINUE
      IF(KPDE.EQ.NPDE)GO TO 150
      RY=    1.0000000000E-03*R(KPDE)
      DY=-    2.0000000000E+01*DRHUV(IST+KPDE)
      FVAL=SP*UPH(KPDE)+DY+RY
      RETURN
  150 CONTINUE
      TL=    4.0000000000E+05*
     * (DRHLM(IC)*UPH(NPDE)+RHLM(IC)*UPH2(NPDE))
      TD=-    2.0000000000E+01*UPH(NPDE)*( +C(IST+ 1)*RHUV(IST+ 1) +
     * C(IST+ 2)*RHUV(IST+ 2))
      TR=-    1.0000000000E-06*( +R( 1)*H(IST+ 1) +R( 2)*H(IST+ 2))
      TX= -2.0000000000E-02*DQX(IC)
      FVAL=SP*UPH(NPDE)+(TL+TR+TD+TX)/CM(IC)
      RETURN
      END
```

```
      PROGRAM LOADF(INPUT,OUTPUT,TAPE5=INPUT,TAPE6=OUTPUT,
     * TAPE3,TAPE9,TAPE15)
C  LOADF CREATES THE SUBROUTINE F IN FLSC.
      DIMENSION II(72)
      DIMENSION LB(25),W(25),AU(7,25),AL(7,25)
      DIMENSION ALO(25),BLU(25),ABD(25,25),BBD(25,25)
      DIMENSION LBPR(25)
      DIMENSION III(44)
      DIMENSION LBROT(25),SGA(25),ESK(25),UM(25),ALP(25),ZROT(25),DF(25)
      DIMENSION AV(25),BV(25)
      WRITE(3,1000)
1000  FORMAT(1HC,2X,34HWE WANT TO AVOID OIVISION BY ZERO.  )
      WRITE(3,1012)
1012  FORMAT(6X,14HOO 5 K=1,NPOEM)
      WRITE(3,1014)
1014  FORMAT(6X,32HIF(ABS(U(K)).LT.SMALL)U(K)=SMALL  )
      WRITE(3,1016)
1016  FORMAT(1X,1H5,4X,36HIF(ABS(UPH(K)).LT.SMALL)UPH(K)=SMALL  )
      REAO(5,12)NLINE
12    FORMAT(10I4)
C  NLINE IS THE NUMBER OF COMMENT LINES TO BE READ AND PRINTED.
      OO 20 K=1,NLINE
      REAO(5,22)II
      WRITE(3,22)II
20    CONTINUE
22    FORMAT(72A1)
24    FORMAT(/1X,72A1/)
      REAO(5,I2)NSPC
      NM=NSPC-1
      LBM=1H-
      LBU=2HU(
      LBP=1H)
      WRITE(3,1020)((LBM,LBU,K,LBP),K=I,NM)
1020  FORMAT(6X,6HYN=1.0,8(A1,A2,I2,A1),A1,2(/5X,1H*,1X,
     *  8(A2,I2,A1,A1))  )
      WRITE(3,1025)
1025  FORMAT(6X,33HCALL RT(U,YN,R,NPOE,KPDE,IC,KSKR) )
      WRITE(3,18)NSPC
18    FORMAT(6X,4HIST=,I2,7H*(IC-1) )
C  ASSUME AT MOST ONE POLAR SPECIES.  (OIPOLE MOMENT NON-ZERO).
C  THEN A* AND B* CAN BE APPROXIMATED BY LENNARD-JONES COLLISION
C  INTEGRALS, EVEN IF THE INPUT PARAMETERS ARE STOCKMAYER.
      DO 30 K=1,NSPC
      READ(5,32)   LB(K),W(K),OF(K),SGA(K),ESK(K),UM(K),ALP(K),ZROT(K),
     * LBROT(K)
      WRITE(6,34)K,LB(K),W(K),OF(K),SGA(K),ESK(K),UM(K),ALP(K),ZROT(K),
     * LBROT(K)
      REAO(15,36)(AU(L,K),L=1,5),(III(L),L=I,5)
      WRITE(6,36)(AU(L,K),L=I,5),(III(L),L=I,5)
      READ(15,36)(AU(L,K),L=6,7),(AL(L,K),L=1,3),(III(L),L=1,5)
      WRITE(6,36)(AU(L,K),L=6,7),(AL(L,K),L=1,3),(III(L),L=I,5)
      READ(15,37)(AL(L,K),L=4,7),(III(L),L=1,20)
      WRITE(6,37)(AL(L,K),L=4,7),(III(L),L=1,20)
30    CONTINUE
32    FORMAT(A5,7F7.0,A5)
34    FORMAT(/2X,I4,4X,A5,4X,7F8.2,4X,A5/)
36    FORMAT(5E15.8,5AI)
```

```
   37   FORMAT(4E15.8,20A1)
        READ(5,232)TPN,PHN,TMN
  232   FORMAT(1P3E12.4)
        WRITE(3,27)
   27   FORMAT(6X,22HIF(KSKT.GT.1)GO TO 100)
        WRITE(3,28)
   28   FORMAT(6X,22HIF(KSKR.GT.1)GO TO 125   )
        READ(5,12)NLINE
        DO 40 K=1,NLINE
        READ(5,22)II
        WRITE(3,22)II
   40   CONTINUE
C  ************************
C  ENTHALPIES AND HEAT CAPACITIES.
C  ************************
        WRITE(3,42)
   42   FORMAT(6X,24HIF(T.GT.1000.)GO TO 2000)
        DO 50 K=1,NSPC
        WRITE(3,52)K,AL(1,K),AL(2,K)
        WRITE(3,54)(AL(L,K),L=3,5)
        WRITE(3,62)K,AL(6,K),AL(1,K)
        WRITE(3,64)AL(2,K),AL(3,K)
        WRITE(3,66)AL(4,K),AL(5,K)
   50   CONTINUE
   52   FORMAT(6X,1HC,I2,9H=1.9872*(,1PE16.8,4H+T*(,1PE16.8)
   54   FORMAT(5X,1H*,1X,3(4H+T*(,1PE16.8),5H)))))
        WRITE(3,56)
   56   FORMAT(6X,10HGO TO 3000)
        WRITE(3,58)
   58   FORMAT(4H2000,2X,8HCONTINUE)
        DO 60 K=1,NSPC
        WRITE(3,52)K,AU(1,K),AU(2,K)
        WRITE(3,54)(AU(L,K),L=3,5)
        WRITE(3,62)K,AU(6,K),AU(1,K)
        WRITE(3,64)AU(2,K),AU(3,K)
        WRITE(3,66)AU(4,K),AU(5,K)
   60   CONTINUE
   62   FORMAT(6X,1HH,I2,9H=1.9872*(,1PE16.8,4H+T*(,1PE16.8)
   64   FORMAT(5X,1H*,1X,4H+T*(,1PE16.8,4H/2.0,4H+T*(,1PE16.8,4H/3.0)
   66   FORMAT(5X,1H*,1X,4H+T*(,1PE16.8,4H/4.0,4H+T*(,1PE16.8,
     * 4H/5.0,6H))))))
        WRITE(3,68)
   68   FORMAT(4H3000,2X,8HCONTINUE)
        WRITE(3,134)
  134   FORMAT(1HC,2X,39HSPECIFIC HEATS AND SPECIFIC ENTHALPIES.   )
        DO 140 K=1,NSPC
        WRITE(3,142)K,K,W(K)
        WRITE(3,144)K,K,W(K)
  140   CONTINUE
  142   FORMAT(6X,6HC(IST+,I2,3H)=C,I2,1H/,F6.2)
  144   FORMAT(6X,6HH(IST+,I2,3H)=H,I2,1H/,F6.2)
        WRITE(3,146)
  146   FORMAT(1X,3H125,2X,8HCONTINUE)
C  ************************
C  THERMAL CONDUCTIVITIES AND BINARY DIFFUSION COEFFICIENTS.
C  READ IN VISCOSITY, THERMAL CONDUCTIVITY, AND BINARY DIFFUSION
C  COEFFICIENTS FROM A FILE CREATED BY VALUES. CY=5.
```

```
C     ************************                              MAIN
      READ(5,12)NLINE                                       MAIN
      DO 72 K=1,NLINE                                       MAIN
      READ(5,22)II                                          MAIN
      WRITE(3,22)II                                         MAIN
72    CONTINUE                                              MAIN
78    FORMAT(1HC,5X,1HV,I2,1H=,1PE14.6,5H*(T**,1PE14.6,1H) ) MAIN
      READ(5,12)NLINE                                       MAIN
      DO 70 K=1,NLINE                                       MAIN
      READ(5,22)II                                          MAIN
      WRITE(3,22)II                                         MAIN
70    CONTINUE                                              MAIN
      DO 80 K=1,NSPC                                        MAIN
      READ(9,82)AV(K),BV(K),III                             MAIN
      WRITE(6,84)K,L8(K),AV(K),BV(K),III                    MAIN
      READ(9,82)ALD(K),BLD(K),III                           MAIN
      WRITE(6,84)K,L8(K),ALD(K),BLD(K),III                  MAIN
80    CONTINUE                                              MAIN
82    FORMAT(1P2E14.6,44A1)                                 MAIN
84    FORMAT(/2X,I4,4X,A4,4X,1P2E14.6,44A1/)                MAIN
      DO 76 K=1,NSPC                                        MAIN
76    WRITE(3,78)K,AV(K),BV(K)                              MAIN
      DO 90 K=1,NSPC                                        MAIN
      WRITE(3,92)K,ALD(K),BLD(K)                            MAIN
90    CONTINUE                                              MAIN
92    FORMAT(6X,2HRL,I2,1H=,1PE14.6,5H*(T**,1PE14.6,1H))    MAIN
      READ(5,12)NLINE                                       MAIN
      DO 100 K=1,NLINE                                      MAIN
      READ(5,22)II                                          MAIN
      WRITE(3,22)II                                         MAIN
100   CONTINUE                                              MAIN
      NM=NSPC-1                                             MAIN
      DO 110 I=1,NSPC                                       MAIN
      DO 110 J=I,NSPC                                       MAIN
      READ(9,82)ABD(I,J),BBD(I,J),III                       MAIN
      WRITE(6,112)I,J,LB(I),LB(J),ABD(I,J),BBD(I,J),III     MAIN
110   CONTINUE                                              MAIN
112   FORMAT(/2X,I4,4X,I4,4X,A4,4X,A4,4X,1P2E14.6,44A1/)    MAIN
      READ(5,114)PRESS                                      MAIN
114   FORMAT(F6.0)                                          MAIN
      WRITE(3,116)PRESS                                     MAIN
      WRITE(6,116)PRESS                                     MAIN
116   FORMAT(1HC,2X,7HPRESS =,F6.2)                         MAIN
      DO 120 I=1,NSPC                                       MAIN
      DO 120 J=I,NSPC                                       MAIN
      ABD(I,J)=ABD(I,J)/PRESS                               MAIN
      WRITE(3,122)I,J,ABD(I,J),BBD(I,J)                     MAIN
120   CONTINUE                                              MAIN
122   FORMAT(6X,1HD,2I2,1H=,1PE14.6,5H*(T**,1PE14.6,1H))    MAIN
C     ************************                              MAIN
C     SPACE DERIVATIVES.                                    MAIN
C     ************************                              MAIN
      LBPL=1H+                                              MAIN
      WRITE(3,148)                                          MAIN
148   FORMAT(1HC,2X,18HSPACE DERIVATIVES.)                  MAIN
      NS=NSPC+1                                             MAIN
      WRITE(3,149)NS                                        MAIN
```

```
 149   FORMAT(6X,4HYS=Y,I2)
       DO 150 K=1,NSPC
       WRITE(3,152)K,K
 150   CONTINUE
 152   FORMAT(6X,1HX,I2,2H=Y,I2,3H/YS)
       DO 160 K=1,NM
       WRITE(3,162)K,K
       WRITE(3,164)K,K
       WRITE(3,166)K,K
 160   CONTINUE
 162   FORMAT(6X,1HU,I2,3H=U(,I2,1H))
 164   FORMAT(6X,2HDU,I2,5H=UPH(,I2,1H))
 166   FORMAT(6X,3HDDU,I2,6H=UPH2(,I2,1H))
       LBU=1HU
       WRITE(3,172)NSPC,((LBM,LBU,K),K=1,NM)
 172   FORMAT(6X,1HU,I2,4H=1.0,8(A1,A1,I2),A1,2(/5X,1H*,1X,
      *  8(A1,I2,A1)) )
       LBDU=2HDU
       WRITE(3,174)NSPC,((LBM,LBDU,K),K=1,NM)
 174   FORMAT(6X,2HDU,I2,1H=,8(A1,A2,I2),A1,2(/5X,1H*,1X,
      *  8(A2,I2,A1)) )
       LBDDU=3HDDU
       WRITE(3,176)NSPC,((LBM,LBDDU,K),K=1,NM)
 176   FORMAT(6X,3HDDU,I2,1H=,8(A1,A3,I2),A1,2(/5X,1H*,1X,
      *  8(A3,I2,A1)) )
       DO 180 K=1,NSPC
       WRITE(3,182)K,K,W(K)
 180   CONTINUE
 182   FORMAT(6X,2HDY,I2,3H=DU,I2,1H/,F6.2)
       LBDY=2HDY
       WRITE(3,186)((LBPL,LBDY,K),K=1,NSPC)
 186   FORMAT(6X,4HDYS=,8(A1,A2,I2),A1,2(/5X,1H*,1X,8(A2,I2,A1)) )
       PSR=PRESS/82.05
       WRITE(3,234)TPN,PHN,TMN
       WRITE(6,234)TPN,PHN,TMN
 234   FORMAT(1HC,2X,5HTPN =,1PE12.4,6X,5HPHN =,1PE12.4,6X,
      * 5HTMN =,1PE12.4)
       WRITE(3,226)TPN
 226   FORMAT(6X,13HDT=UPH(NPDE)*,1PE12.4)
       WRITE(3,242)PSR
 242   FORMAT(6X,5HORH=-,1PE18.10,21H*(DT/T+DYS/YS)/(T*YS))
       WRITE(3,1202)
 1202  FORMAT(6X,16HDYSY=DYS/(YS*YS) )
       DO 1250 K=1,NSPC
       WRITE(3,1204)K,K,K
 1204  FORMAT(6X,2HOX,I2,3H=DY,I2,5H/YS-Y,I2,5H*DYSY )
       A=ALO(K)*BLO(K)
       B=BLD(K)-1.0
       WRITE(3,1208)K,A,B
 1208  FORMAT(6X,2HDL,I2,1H=,1PE20.12,6H*(T**(,1PE14.6,5H))*DT )
       RG=1.9872
       A=15.0*RG*AV(K)/(4.0*W(K))
       B=BV(K)
       WRITE(3,1212)K,A,B
 1212  FORMAT(6X,3HRLZ,I2,1H=,1PE20.12,6H*(T**(,1PE14.6,2H)) )
       A=A*B
       B=B-1.0
```

```
      WRITE(3,1216)K,A,B
 1216 FORMAT(6X,3HDLZ,12,1H=,1PE20.12,6H*(T**(,1PE14.6,2H)),3H*DT )
      A=ABD(K,K)*BBD(K,K)
      B=BBD(K,K)-1.0
      WRITE(3,1220)K,K,A,B
 1220 FORMAT(6X,2HDD,2I2,1H=,1PE20.12,6H*(T**(,1PE14.6,5H))*DT )
      A=1.0/AV(K)
      B=-BV(K)
      WRITE(3,1224)K,A,B
 1224 FORMAT(6X,2HVV,12,1H=,1PE20.12,6H*(T**(,1PE14.6,2H)) )
      A=A*B
      B=B-1.0
      WRITE(3,1228)K,A,B
 1228 FORMAT(6X,3HDVV,12,1H=,1PE20.12,6H*(T**(,1PE14.6,5H))*DT )
      WRITE(3,1232)K,K,K,K
 1232 FORMAT(6X,4HXXSV,12,2H=X,12,2H*X,I2,3H*VV,12)
      WRITE(3,1236)K,K,K,K,K,K,K
 1236 FORMAT(6X,5HDXXSV,I2,6H=2.0*X,I2,3H*DX,12,3H*VV,I2,2H+X,12,2H*X,
     * I2,4H*DVV,I2)
 1250 CONTINUE
      DO 1300 I=1,NM
      IP=I+1
      DO 1300 J=IP,NSPC
      A=1.0/ABD(I,J)
      B=-BBD(I,J)
      WRITE(3,1258)I,J,A,B
 1258 FORMAT(6X,2HVD,2I2,1H=,1PE20.12,6H*(T**(,1PE14.6,2H)) )
      A=A*B
      B=B-1.0
      WRITE(3,1262)I,J,A,B
 1262 FORMAT(6X,3HDVD,2I2,1H=,1PE20.12,6H*(T**(,1PE14.6,5H))*DT )
      WRITE(3,1268)((I,J),L=1,3)
 1268 FORMAT(6X,4HXXSD,2I2,2H=X,I2,2H*X,I2,3H*VD,2I2)
      WRITE(3,1274)((I,J),L=1,7)
 1274 FORMAT(6X,5HDXXSD,2I2,3H=DX,12,2H*X,12,3H*VD,2I2,2H+X,I2,
     * 3H*DX,I2,3H*VD,2I2,2H+X,I2,2H*X,I2,4H*DVD,2I2)
      WRITE(3,1278)I,J,I,J
 1278 FORMAT(6X,5HXXTSD,2I2,5H=XXSD,2I2,2H*T)
      WRITE(3,1282)((I,J),L=1,3)
 1282 FORMAT(6X, 5HDXTSD,2I2,6H=DXXSD,2I2,7H*T+XXSD,2I2,3H*DT)
 1300 CONTINUE
C    ***********************
C    SPECIFIC HEAT OF THE MIXTURE.
C    ***********************
      WRITE(3,124)
 124  FORMAT(1HC,2X,44HSPECIFIC HEAT OF THE MIXTURE.  NTIS FORMULA. )
      LBC=6HC(IST+
      LBU=3H)*U
      WRITE(3,132)((LBPL,LBC,K,LBU,K),K=1,NSPC)
 132  FORMAT(6X,7HCM(IC)=,4(A1,A6,12,A3,I2),A1,
     * 4(/5X,1H*,1X,4(A6,I2,A3,I2,A1)) )
C    ***********************
C    THERMAL CONDUCTIVITY OF THE MIXTURE.
C    ***********************
C    BOLTZMAN CONSTANT.
      RK=1.38054E-16
      WRITE(3,272)
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      WRITE(3,274)
  272 FORMAT(1HC,2X,36HTHERMAL CONDUCTIVITY OF THE MIXTURE.)
  274 FORMAT(1HC,2X,35HHIRSHFELDER METHOD FOR MONATOMICS.    )
      WRITE(3,276)
  276 FORMAT(1HC,2X,39HP. 37A, TOULOUKIEN, LILEY, AND SAXENA.    )
      WRITE(3,277)
  277 FORMAT(1HC,2X,69HNOTE IN THE FORMULA, LAMBDA MUST BE IN THE SAME U
     *NITS AS D*P/T.                  )
      WRITE(3,278)
  278 FORMAT(1HC,2X,63HLAMBDA=15*R*VISC/(4*M), WHERE R=82.05 CM**3-ATM/M
     *OLE-K.                 )
      WRITE(3,279)
  279 FORMAT(1HC,2X,69HTO CONVERT LAMBDA BACK TO CAL/CM-SEC-K, MULTIPLY
     *BY 1.9872/82.05.                     )
      READ(5,82)AAST,BAST,III
      WRITE(6,123)AAST,BAST,III
  123 FORMAT(/2X,1P2E14.6,44A1)
      READ(5,82)  ABST,BBST,III
      WRITE(6,123)ABST,BBST,III
      WRITE(3,282)BAST
  282 FORMAT(6X,11HTASTLJ=T**(,1PE14.6,1H) )
      WRITE(3,284)BBST
  284 FORMAT(6X,11HTBSTLJ=T**(,1PE14.6,1H) )
      BM=BAST-1.0
      WRITE(3,1382)BAST,BM
 1382 FORMAT(6X,6HDTAST=,1PE14.6,8H*DT*T**(,1PE14.6,1H) )
      BM=BBST-1.0
      WRITE(3,1384)BBST,BM
 1384 FORMAT(6X,6HDTBST=,1PE14.6,8H*DT*T**(,1PE14.6,1H) )
      DO 280 I=1,NM
      IP=1+I
      DO 280 J=IP,NSPC
      A=16.0*W(I)*W(J)/(25.0*(W(I)+W(J))*(W(I)+W(J))*PRESS)
      B=13.75
      ESKIJ=SQRT(ESK(I)*ESK(J))
      IF(UM(I).EQ.0.0.AND.UM(J).EQ.0.0)GO TO 287
C  COMBINING RULE.  P. 528, REID AND SHERWOOD.
      IF(UM(I).NE.0.0)LP=I
      IF(UM(J).NE.0.0)LP=J
      IF(LP.EQ.I)LNP=J
      IF(LP.EQ.J)LNP=I
      UMP=UM(LP)*1.0E-18
      SGC=SGA(LP)*1.0E-8
      TPSTAR=UMP*UMP/(ESK(LP)*RK*SGC*SGC*SGC*SQRT(8.0))
      FC=1.0+(1.0/SQRT(2.0))*(ALP(LNP)*TPSTAR/(SGA(LNP)**3))*
     * SQRT(ESK(LP)/ESK(LNP))
      WRITE(6,1234)I,J,LP,LNP,FC
 1234 FORMAT(4I4,1PE12.4)
      ESKIJ=ESKIJ*FC*FC
  287 CONTINUE
      C=3.0*ABST/(ESKIJ**BBST)
      D=4.0*AAST/(ESKIJ**BAST)
      AB=A*B
      AC=A*C
      AD=A*D
      WRITE(3,286)AB,AC,AD
  286 FORMAT(6X,5HCNST=,1PE20.12,1H-,1PE20.12,1H*,/5X,1H*,1X,
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```
     * 7HTBSTLJ-,1PE20.12,7H*TASTLJ)                                  MAIN
       WRITE(3,1386)AC,AD                                              MAIN
 1386  FORMAT(6X,6HDCNST=,1H-,1PE20.12,1H*,6HDTBST-,1PE20.12,6H*DTAST) MAIN
       WRITE(3,288)I,J,I,J                                             MAIN
 288   FORMAT(6X,2HZ(,I2,1H,,I2,12H)=CNST*XXTSD,2I2)                   MAIN
       WRITE(3,290)I,J,I,J,I,J                                         MAIN
 290   FORMAT(6X,2HDZ,I2,1HS,I2,11H=CNST*DXTSD,2I2,                    MAIN
     * 12H+DCNST*XXTSD,2I2 )                                           MAIN
       WRITE(3,292)J,I,I,J                                             MAIN
 292   FORMAT(6X,2HZ(,I2,1H,,I2,4H)=Z(,I2,1H,,I2,1H) )                 MAIN
       WRITE(3,294)J,I,I,J                                             MAIN
 294   FORMAT(6X,2HDZ,I2,1HS,I2,3H=DZ,I2,1HS,I2)                       MAIN
 280   CONTINUE                                                        MAIN
       DO 300 I=1,NSPC                                                 MAIN
       DO 295 K=1,NSPC                                                 MAIN
       IF(I.EQ.K)GO TO 295                                             MAIN
       IMIN=MIN0(I,K)                                                  MAIN
       IMAX=MAX0(I,K)                                                  MAIN
       C=16.0/(25.0*(W(I)+W(K))*(W(I)+W(K))*PRESS)                     MAIN
       D=7.5*W(I)*W(I)+6.25*W(K)*W(K)                                  MAIN
       ESKIK=SQRT(ESK(I)*ESK(K))                                       MAIN
       IF(UM(I).EQ.0.0.AND.UM(K).EQ.0.0)GO TO 299                      MAIN
C  COMBINING RULE.  P. 528, REID AND SHERWOOD.                         MAIN
       IF(UM(I).NE.0.0)LP=I                                            MAIN
       IF(UM(K).NE.0.0)LP=K                                            MAIN
       IF(LP.EQ.I)LNP=K                                                MAIN
       IF(LP.EQ.K)LNP=I                                                MAIN
       UMP=UM(LP)*1.0E-18                                              MAIN
       SGC=SGA(LP)*1.0E-8                                              MAIN
       TPSTAR=UMP*UMP/(ESK(LP)*RK*SGC*SGC*SGC*SQRT(8.0))               MAIN
       FC=1.0+(1.0/SQRT(2.0))*(ALP(LNP)*TPSTAR/(SGA(LNP)**3))*         MAIN
     * SQRT(ESK(LP)/ESK(LNP))                                          MAIN
       WRITE(6,1234)I,J,LP,LNP,FC                                      MAIN
       ESKIK=ESKIK*FC*FC                                               MAIN
 299   CONTINUE                                                        MAIN
       E=3.0*W(K)*W(K)*ABST/(ESKIK**BBST)                              MAIN
       F =4.0*W(I)*W(K)*AAST/(ESKIK**BAST)                             MAIN
       CD=C*D                                                          MAIN
       CE=C*E                                                          MAIN
       CF=C*F                                                          MAIN
       WRITE(3,296)CD,CE,CF                                            MAIN
 296   FORMAT(6X,6HCNST=-,1PE20.12,1H+,1PE20.12,1H*,/5X,1H*,1X,        MAIN
     * 7HTBSTLJ-,1PE20.12,7H*TASTLJ )                                  MAIN
       WRITE(3,1396)CE,CF                                              MAIN
 1396  FORMAT(6X,6HDCNST=,1PE20.12,1H*,6HDTBST-,1PE20.12,6H*DTAST)     MAIN
       WRITE(3,297)K,IMIN,IMAX                                         MAIN
 297   FORMAT(6X,1HT,I2,7H=-XXTSD,2I2,5H*CNST)                         MAIN
       WRITE(3,298)K,IMIN,IMAX,IMIN,IMAX                               MAIN
 298   FORMAT(6X,2HDT,I2,7H=-DXTSD,2I2,5H*CNST,6H-XXTSD,2I2,6H*DCNST ) MAIN
 295   CONTINUE                                                        MAIN
       LBBL=1H                                                         MAIN
       LBT=1HT                                                         MAIN
C  GAS CONSTANT IN CM**3-ATM/MOLE-K.                                   MAIN
       RGA=82.05                                                       MAIN
       A=-16.0*W(I)/(15.0*RGA)                                         MAIN
       WRITE(3,302)I,I,A,1                                             MAIN
 302   FORMAT(6X,2HZ(,I2,1H,,I2,2H)=,1PE20.12,5H*XXSV,I2,1H-)          MAIN
```

```
      LBLP=1H(
      IF(I.EQ.I)WRITE(3,304)LBLP,((LBBL,LBPL,LBT,K),K=2,NSPC),LBP
  304 FORMAT(5X,1H*,IX,2AI,10(2A1,I2,A1),A1,/5X,IH*,IX,10(2AI,I2,A1)   )
      IF(1.EQ.NSPC)WRITE(3,304)LBLP,((LBBL,LBPL,LBT,K),K=1,NM),LBP
      IF(1.EQ.1.OR.1.EQ.NSPC)GO TO 307
      IM=1-1
      IP=1+1
      WRITE(3,304)LBLP,((LBBL,LBPL,LBT,K),K=1,1M),((LBBL,LBPL,LBT,K),
     * K=IP,NSPC),LBP
  307 CONTINUE
      WRITE(3,305)1,I,A,1
  305 FORMAT(6X,2HDZ,12,1HS,12,IH=,1PE20.12,6H*DXXSV,I2,1H- )
      LBDT=2HDT
      IF(I.EQ.1)WRITE(3,306)LBLP,((LBBL,LBPL,LBDT,K),K=2,NSPC),LBP
  306 FORMAT(5X,1H*,IX,2AI,10(AI,A2,12,A1),AI,/5X,IH*,1X,
     * 10(A1,A2,I2,A1 ) )
      IF(I.EQ.NSPC)WRITE(3,306)LBLP,((LBBL,LBPL,LBDT,K),K=1,NM),LBP
      IF(1.EQ.1.OR.I.EQ.NSPC)GO TO 309
      IM=1-1
      IP=1+I
      WRITE(3,306)LBLP,((LBBL,LBPL,LBDT,K),K=1,IM),((LBBL,LBPL,LBOT,K),
     * K=1P,NSPC),LBP
  309 CONTINUE
  300 CONTINUE
      DO 310 K=1,NSPC
      WRITE(3,312)K,K
  310 CONTINUE
  312 FORMAT(6X,2HV(,I2,3H)=X,12)
      NDIM=20
      WRITE(3,428)NSPC,NOIM
      WRITE(3,432)NSPC,NDIM
      LBX=IHX
      LBV=3H*V(
C   CONVERT RLM FROM CM**3-ATM/CM-SEC-K TO CAL/CM-SEC-K.
      A=-4.0*RG/RGA
      WRITE(3,316)A,((LBBL,LBPL,LBX,K,LBV,K,LBP),K=I,NSPC),LBP
  316 FORMAT(6X,4HRLM=,1PE14.6,2H*(,4(3A1,12,A3,I2,A1),2AI,2(/5X,IH*,1X,
     * 5(AI,12,A3,12,3A1)) )
      LBDZ=2HOZ
      LBV=3H*V(
      LBP=1H)
      LBS=IHS
      LBSP=1HS
      DO 320 1=1,NSPC
      WRITE(3,322)1,1,((LBM,LBDZ,1,LBS,J,LBV,J,LBP),J=1,NSPC)
  320 CONTINUE
  322 FORMAT(6X,3HDV(,12,4H)=0X,12,3(A1,A2,12,A1,12,A3,12,A1),A1,
     * 5(/5X,1H*,1X,4(A2,12,A1,I2,A3,12,2A1)) )
      WRITE(3,546)NSPC,NDIM
      LBBL=IH
      LBX=1HX
      LBDV=4H*DV(
      LBDX=2HOX
      LBV=3H*V(
      WRITE(3,326)A,((L BL,LBPL,LBX,K,LBDV,K,LBP,LBPL,LBDX,K,LBV,K,LBP)
     * ,K=1,NSPC),LBP
  326 FORMAT(6X,5HDRLM=,1PE14.6,2H*(, A1,12,A4,12,2A1,A2,I2,A3,12,A1,
```

```
     * 2A1,10(/5X,1H*,1X,2(A1,12,A4,I2,2AI,A2,I2,A3,12,3AI)) )
C  THE ABOVE IS THE THERMAL CONDUCTIVITY FOR A MIXTURE OF MONATOMIC
C  GASES.  COMPUTE THE CORRECTION FACTOR FOR POLYATOMIC GASES.
      I=I
      LBX=IHX
      LBVD=3H*VD
      LBDX=2HDX
      LBDVD=4H*DVD
      IF(DF(I).EQ.0.0)GO TO 725
      WRITE(3,702)((LBPL,LBX,J,LBVD,I,J),J=2,NSPC)
702   FORMAT(6X,4HSUM=,5(2AI,12,A3,2I2),A1,3(/5X,1H*,IX,
     * 5(A1,I2,A3,2I2,A1)) )
      WRITE(3,706)((LBPL,LBDX,J,LBVD,1,J,LBPL,LBX,J,LBDVD,I,J),J=2,NSPC)
706   FORMAT(6X,5HDSUM=,2(AI,A2,12,A3,2I2,2A1,12,A4,2I2),AI,
     * 9(/5X,1H*,1X,2(A2,I2,A3,2I2,2A1,12,A4,2I2,AI)) )
      WRITE(3,7I0)1,1,1
7I0   FORMAT(6X,6HB=I.0+,1HD,2I2,6H*SUM/X,12)
      WRITE(3,714)((I),L=1,11)
714   FORMAT(6X,5HDB=DD,2I2,6H*SUM/X,12,2H+D,2I2,7H*DSUM/X,12,
     * 2H-D,2I2,7H*SUM*DX,I2,3H/(X,12,2H*X,I2,1H) )
      WRITE(3,7I8)I,I
718   FORMAT(6X,11HRLM=RLM+(RL,12,4H-RLZ,12,3H)/B )
      WRITE(3,722)I,1,I,1
722   FORMAT(6X,13HDRLM=DRLM+(DL,I2,4H-DLZ,I2,5H)/B-(,2HRL,I2,4H-RLZ,
     * I2,I0H)*DB/(B*B) )
725   CONTINUE
      DO 730 I=2,NM
      IF(DF(I).EQ.0.0)GO TO 730
      IM=I-1
      IP=I+I
      WRITE(3,702)((LBPL,LBX,J,LBVD,J,I),J=I,IM),
     * ((LBPL,LBX,J,LBVD,I,J),J=IP,NSPC)
      WRITE(3,706)((LBPL,LBDX,J,LBVD,J,I,LBPL,LBX,J,LBDVD,J,1),J=I,1M),
     * ((LBPL,LBDX,J,LBVD,1,J,LBPL,LBX,J,LBDVD,1,J),J=IP,NSPC)
      WRITE(3,710)I,I,1
      WRITE(3,714)((I),L=I,1I)
      WRITE(3,7I8)1,I
      WRITE(3,722)1,I,I,1
730   CONTINUE
      I=NSPC
      IF(DF(1).EQ.0.0)GO TO 735
      WRITE(3,702)((LBPL,LBX,J,LBVD,J,1),J=I,NM)
      WRITE(3,706)((LBPL,LBDX,J,LBVD,J,I,LBPL,LBX,J,LBDVD,J,1),J=I,NM)
      WRITE(3,710)1,1,I
      WRITE(3,7I4)((I),L=1,11)
      WRITE(3,718)1,1
      WRITE(3,722)1,1,I,I
735   CONTINUE
      WRITE(3,738)
738   FORMAT(6X,15HRHLM(IC)=RH*RLM)
      WRITE(3,742)
742   FORMAT(6X,25HDRHLM(IC)=RH*DRLM+DRH*RLM )
C  *************************
C  SOLVE FOR UV.
C  *************************
      WRITE(3,400)
400   FORMAT(1HC,2X,I3HSOLVE FOR UV.)
```

```
      WRITE(3,402)NSPC
  402 FORMAT(6X,2HV(,I2,5H)=0.0 )
      DO 405 K=1,NM
      WRITE(3,408)K,K,PHN
  405 CONTINUE
  408 FORMAT(6X,2HV(,I2,4H)=DX,I2,4H*RH/,1PE12.4 )
      DO 410 K=1,NSPC
      WRITE(3,412)NSPC,K,K
      WRITE(3,414)NSPC,K,K
  410 CONTINUE
  412 FORMAT(6X,2HZ(,I2,1H,,I2,3H)=U,I2)
  414 FORMAT(6X,2HDZ,I2,1HS,I2,3H=DU,I2)
      DO 415 I=1,NM
      IP=I+1
      DO 415 J=IP,NSPC
      WRITE(3,416)I,J,I,J
  416 FORMAT(6X,2HZ(,I2,1H,,I2,6H)=XXSD,2I2)
      IF(J.NE.NSPC)WRITE(3,416)J,I,I,J
      WRITE(3,418)I,J,I,J
  418 FORMAT(6X,2HDZ,I2,1HS,I2,6H=DXXSD,2I2)
      IF(J.NE.NSPC)WRITE(3,418)J,I,I,J
  415 CONTINUE
      I=1
      LBXXSD=4HXXSD
      WRITE(3,422)I,I,((LBM,LBXXSD,I,J),J=2,NSPC)
  422 FORMAT(6X,2HZ(,I2,1H,,I2,2H)=,4(A1,A4,2I2),A1,
     * 3(/5X,1H*,1X,5(A4,2I2,A1)) )
      LBD=5HDXXSD
      WRITE(3,424)I,I,((LBM,LBD,I,J),J=2,NSPC)
  424 FORMAT(6X,2HDZ,I2,1HS,I2,1H=,4(A1,A5,2I2),A1,
     *  3(/5X,1H*,1X,5(A5,2I2,A1)) )
      DO 420 I=2,NM
      IM=I-1
      IP=I+1
      WRITE(3,422)I,I,((LBM,LBXXSD,J,I),J=1,IM),
     * ((LBM,LBXXSD,I,J),J=IP,NSPC)
      WRITE(3,424)I,I,((LBM,LBD,J,I),J=1,IM),((LBM,LBD,I,J),J=IP,NSPC)
  420 CONTINUE
      WRITE(3,428)NSPC,NDIM
  428 FORMAT(6X,9HCALL DEC(,I2,1H,,I2,11H,Z,IPS,IER) )
      WRITE(3,432)NSPC,NDIM
  432 FORMAT(6X,9HCALL SOL(,I2,1H,,I2,9H,Z,V,IPS) )
      DO 435 K=1,NSPC
      WRITE(3,438)K,K,K
  435 CONTINUE
  438 FORMAT(6X,2HUV,I2,2H=U,I2,3H*V(,I2,1H) )
      DO 440 K=1,NSPC
      WRITE(3,442)K,K
  440 CONTINUE
  442 FORMAT(6X,9HRHUV(IST+,I2,7H)=RH*UV,I2)
C     ************************
C     SOLVE FOR THE SPACE DERIVATIVE OF UV.
C     ************************
      WRITE(3,522)
  522 FORMAT(1HC,2X,30HSPACE DER OF DENSITY TIMES UV.)
      DO 500 K=1,NSPC
      WRITE(3,502)K,K,W(K)
```

```
 500  CONTINUE
 502  FORMAT(6X,3HDDY,I2,4H=DDU,I2,IH/,F6.2)
      LBDDY=3HDDY
      WRITE(3,506)((LBPL,LBDDY,K),K=I,NSPC)
 506  FORMAT(6X,5HDDYS=,8(A1,A3,I2),A1,2(/5X,1H*,1X,8(A3,I2,AI)) )
      WRITE(3,510)
 510  FORMAT(6X,I8HDYSYSQ=(DYS/YS)**2 )
      DO 515 K=I,NSPC
      WRITE(3,518)K,K,K,K,K
 515  CONTINUE
 518  FORMAT(6X,3HDDX,I2,5H=(DDY,I2,7H-2.0*DY,I2,I3H*DYS/YS+2.0*Y,
     * I2,9H*DYSYSQ-Y,I2,12H*DDYS/YS)/YS  )
      LBDZ=2HDZ
      LBV=3H*V(
      LBS=IHS
      LBSP=IHS
      DO 525 I=1,NM
      WRITE(3,528)I,I,I,PHN,((LBM,LBDZ,I,LBS,J,LBV,J,LBP),J=1,NSPC)
 525  CONTINUE
 528  FORMAT(6X,3HDV(,I2,9H)=(RH*DDX,I2,7H+DRH*DX,I2,2H)/,
     * 1PE12.4,A1,A2,I2,AI,I2,A3,I2,2A1,5(/5X,1H*,1X,
     * 4(A2,I2,A1,I2,A3,I2,2A1)) )
      I=NSPC
      WRITE(3,532)I,((LBM,LBDZ,I,LBSP,J,LBV,J,LBP),J=1,NSPC)
 532  FORMAT(6X,3HDV(,I2,2H)=,3(AI,A2,I2,AI,I2,A3,I2,AI),AI,
     * 5(/5X,IH*,1X,4(A2,I2,AI,I2,A3,I2,2AI)) )
      WRITE(3,546)NSPC,NDIM
 546  FORMAT(6X,9HCALL SOL(,I2,IH,,I2,10H,Z,DV,IPS) )
      DO 550 K=I,NSPC
      WRITE(3,552)K,K,K,K,K
 550  CONTINUE
 552  FORMAT(6X,3HDUV,I2,2H=U,I2,4H*DV(,I2,4H)+DU,I2,3H*V(,I2,IH) )
      DO 8I0 K=1,NSPC
      WRITE(3,8I2)K,K,K
 8I0  CONTINUE
 812  FORMAT(6X,10HDRHUV(IST+,I2,8H)=DRH*UV,I2,7H+RH*DUV,I2)
C ************************
C FIND THE TIME DERIVATIVES.
C ************************
      WRITE(3,612)
 6I2  FORMAT(IHC,2X,26HFIND THE TIME DERIVATIVES.)
      WRITE(3,622)
 622  FORMAT(6X,I5HSP=ASP+BSP*TIME)
      TMSPH2=TMN/(PHN*PHN)
      WRITE(3,628)
 628  FORMAT(1X,3HI00,2X,8HCONTINUE)
      WRITE(3,632)
 632  FORMAT(6X,25HIF(KPDE.EQ.NPDE)GO TO I50)
      WRITE(3,636)TMN
 636  FORMAT(6X,3HRY=,1PE20.10,8H*R(KPDE) )
      TMSPH=TMN/PHN
      WRITE(3,638)TMSPH
 638  FORMAT(6X,4HDY=-,1PE20.10,16H*DRHUV(IST+KPDE)  )
      WRITE(3,642)
 642  FORMAT(6X,23HFVAL=SP*UPH(KPDE)+DY+RY)
      WRITE(3,646)
 646  FORMAT(6X,6HRETURN)
```

```
          WRITE(3,648)
  648     FORMAT(1X,3H150,2X,8HCONTINUE)
          WRITE(3,662)TMSPH2
  662     FORMAT(6X,3HTL=,1PE20.10,1H*)
          WRITE(3,664)
  664     FORMAT(5X,1H*,1X,41H(DRHLM(IC)*UPH(NPDE)+RHLM(IC)*UPH2(NPDE)) )
          LBBL=1H
          LBC=6HC(IST+
          LBRHUV=10H)*RHUV(IST
          WRITE(3,668)TMSPH,((LBBL,LBPL,LBC,K,LBRHUV,LBPL,K,LBP),K=1,NSPC)
         * ,LBP
  668     FORMAT(6X,4HTD=-,1PE20.10,12H*UPH(NPDE)*(,2A1,A6,I2,A10,A1,I2,3A1,
         * 10(/5X,1H*,1X,2(A6,I2,A10,A1,I2,3A1)) )
          TMSTP=TMN/TPN
          LBR=2HR(
          LBH=8H)*H(IST+
          WRITE(3,672)TMSTP,((LBBL,LBPL,LBR,K,LBH,K,LBP),K=1,NSPC),LBP
  672     FORMAT(6X,4HTR=-,1PE20.10,2H*(,2(2A1,A2,I2,A8,I2,A1),2A1,
         * 9(/5X,1H*,1X,2(A2,I2,A8,I2,3A1)) )
          WRITE(3,676)
  676     FORMAT(6X,35HFVAL=SP*UPH(NPDE)+(TL+TR+TD)/CM(IC) )
          STOP
          END
```

```
PROGRAM  WILL BE ENTERED AT  LOADF      (   241)                    SCM LENGTH     20275          LCM LENGTH        0

         BLOCK         ADDRESS     LENGTH       FILE

         LOADF           110       12777        LGO
          /STP.END/     13107          1       SL-FTNLIB
          /FCL.C./      13110         30       SL-FTNLIB
          /Q8.IO./      13140        144       SL-FTNLIB
         Q2NTRY=        13304          4       SL-FTNLIB
         CUMIO=         13310         10       SL-FTNLIB
         FECMSK=        13320         41       SL-FTNLIB
         FEIFST=        13361          3       SL-FTNLIB
         FLTIN=         13364        156       SL-FTNLIB
         FLTOUT=        13542        315       SL-FTNLIB
         FMTAP=         14057        377       SL-FTNLIB
         FORSYS=        14456        300       SL-FTNLIB
         FORUTL=        14756         45       SL-FTNLIB
         GETFIT=        15023         54       SL-FTNLIB
         INCOM=         15077        144       SL-FTNLIB
         INPC=          15243        173       SL-FTNLIB
         KODER=         15436        476       SL-FTNLIB
         KRAKER=        16134        454       SL-FTNLIB
         OUTC=          16610        155       SL-FTNLIB
         OUTCOM=        16765        204       SL-FTNLIB
         ERRCAP=        17171        317       SL-FTNLIB
         FERCAP=        17510        171       SL-FTNLIB
         ALOG.          17701         63       SL-FTNLIB
         EXP.           17764         73       SL-FTNLIB
         EXP.MSG        20057         16       SL-FTNLIB
         SQRT           20075          6       SL-FTNLIB
         SQRT.          20103         32       SL-FTNLIB
         SYSAID=        20135          1       SL-FTNLIB
         SYS=1ST        20136         65       SL-FTNLIB
         SYS=AID        20223          7       SL-FTNLIB
         XTOY*          20232         11       SL-FTNLIB
         XTOY.          20243         32       SL-FTNLIB

    1    H2          2.00      2.00      2.92     38.00      0.00      .79   280.00     CNST

 .31001901E+01  .51119464E-03  .52644210E-07 -.34909973E-10  .36945345E-14   H2
-.87738042E+03 -.19629421E+01  .30574451E+01  .26765200E-02 -.58099162E-05   H2
 .55210391E-08 -.18122739E-11 -.98890474E+03 -.22997056E+01                  H2

    2    N2         28.00      2.00      3.62     97.50      0.00     0.00    15.70     VAR

 .28963194E+01  .15154866E-02 -.57235277E-06  .99807393E-10 -.65223555E-14   N2
-.90586184E+03  .61615148E+01  .36748261E+01 -.12081500E-02  .23240102E-05   N2
-.63217559E-09 -.22577253E-12 -.10611588E+04  .23580424E+01                  N2

    1    H2        2.188700E-06  6.502900E-01    H2     VISCOSITY.

    1    H2        6.357900E-06  7.383300E-01    H2     THERMAL CONDUCTIVITY.

    2    N2        4.266700E-06  6.613600E-01    N2     VISCOSITY.

    2    N2        6.407700E-07  7.999600E-01    N2     THERMAL CONDUCTIVITY.
```

```
1     1   H2   H2     1.119300E-04  1.661400E+00   H2    H2    BINARY DIFFUSION.

1     2   H2   N2     5.951700E-05  1.663800E+00   H2    N2    BINARY DIFFUSION.

2     2   N2   N2     1.537400E-05  1.672900E+00   N2    N2    BINARY DIFFUSION.
PRESS =  1.00
TPN =  1.0000E+03      PHN =  5.0000E-05      TMN =  1.0000E-03

 1.088500E+00  9.055700E-03     A*  P. 1128, HIRSHFELDER, ET. AL.

 1.129600E+00 -1.022500E-02     B*  P. 1128, HIRSHFELDER, ET. AL.
```

```
      SUBROUTINE F(TIME,PH,U,UPH,UPH2,FVAL,NPDE,KPDE,IC,KSKT,KSKR)
      DIMENSION Z(20,20),IPS(20)
      DIMENSION V(20),DV(20)
      DIMENSION U(NPDE),UPH(NPDE),UPH2(NPDE)
      COMMON/TABAB/ASP,BSP,TPN,PHN,TMN,TMSPH,TMSPH2,TMSTP,TPENT
      COMMON/TABP/PRESS,PSR,NPDEM
      COMMON/TABSM/SMALL
      COMMON/TABAM/YAB,WAB
      DIMENSION R(20)
      DIMENSION C(1000),H(1000),RHLM(100),ORHLM(100),CM(100)
      COMMON/TABCT/RL,CPMX,HO(20),R2D(20),R2DM(20)
      COMMON/TABMF/RHUV(1000),ORHUV(1000)
      COMMON/TABRY/T,RH,Y1,Y2,Y3,Y4,Y5,Y6,Y7,Y8,Y9,Y10
C  AT EACH CALL THE TIME RATE OF CHANGE FOR ONE PDE IS RETURNED IN FVAL.
C  WE WANT TO AVOID DIVISION BY ZERO.
      DO 5 K=1,NPDEM
      IF(ABS(U(K)).LT.SMALL)U(K)=SMALL
    5 IF(ABS(UPH(K)).LT.SMALL)UPH(K)=SMALL
C  TEST CASE.  BINARY MIX OF H2 AND N2.  TRANSPORT WARNATZ PAR.
C  U = MASS FRACTIONS.  Y = MASS FRACTIONS / MOLECULAR WEIGHTS.
      YN=1.0-U( 1)
      CALL RT(U,YN,R,NPDE,KPDE,IC,KSKR)
      IST= 2*(IC-1)
      IF(KSKT.GT.1)GO TO 100
      IF(KSKR.GT.1)GO TO 125
C  NTIS ENTHALPIES AND HEAT CAPACITIES.
      IF(T.GT.1000.)GO TO 2000
      C 1=1.9872*(  3.05744510E+00+T*(  2.67652000E-03
     * +T*( -5.80991620E-06+T*(  5.52103910E-09+T*( -1.81227390E-12)))))
      H 1=1.9872*( -9.88904740E+02+T*(  3.05744510E+00
     * +T*(  2.67652000E-03/2.0+T*( -5.80991620E-06/3.0
     * +T*(  5.52103910E-09/4.0+T*( -1.81227390E-12/5.0))))))
      C 2=1.9872*(  3.67482610E+00+T*( -1.20815000E-03
     * +T*(  2.32401020E-06+T*( -6.32175590E-10+T*( -2.25772530E-13)))))
      H 2=1.9872*( -1.06115880E+03+T*(  3.67482610E+00
     * +T*( -1.20815000E-03/2.0+T*(  2.32401020E-06/3.0
     * +T*( -6.32175590E-10/4.0+T*( -2.25772530E-13/5.0))))))
      GO TO 3000
 2000 CONTINUE
      C 1=1.9872*(  3.10019010E+00+T*(  5.11194640E-04
     * +T*(  5.26442100E-08+T*( -3.49099730E-11+T*(  3.69453450E-15)))))
      H 1=1.9872*( -8.77380420E+02+T*(  3.10019010E+00
     * +T*(  5.11194640E-04/2.0+T*(  5.26442100E-08/3.0
     * +T*( -3.49099730E-11/4.0+T*(  3.69453450E-15/5.0))))))
      C 2=1.9872*(  2.89631940E+00+T*(  1.51548660E-03
     * +T*( -5.72352770E-07+T*(  9.98073930E-11+T*( -6.52235550E-15)))))
      H 2=1.9872*( -9.05861840E+02+T*(  2.89631940E+00
     * +T*(  1.51548660E-03/2.0+T*( -5.72352770E-07/3.0
     * +T*(  9.98073930E-11/4.0+T*( -6.52235550E-15/5.0))))))
 3000 CONTINUE
C  SPECIFIC HEATS AND SPECIFIC ENTHALPIES.
      C(IST+ 1)=C 1/  2.00
      H(IST+ 1)=H 1/  2.00
      C(IST+ 2)=C 2/ 28.00
      H(IST+ 2)=H 2/ 28.00
  125 CONTINUE
C  VISCOSITY FROM WARNATZ ST PAR.
```

```
C  LEAST SQUARES FIT,  T=300,2000.
C  THERMAL CONDUCTIVITIES FROM WARNATZ ST PAR.
C  LEAST SQUARES FIT,  T=300,2000.
C     V 1=  2.188700E-06*(T**  6.502900E-01)
C     V 2=  4.266700E-06*(T**  6.613600E-01)
      RL 1=  6.357900E-06*(T**  7.383300E-01)
      RL 2=  6.407700E-07*(T**  7.999600E-01)
C  BINARY DIFFUSION COEFFICIENTS FROM WARNATZ ST PAR.
C  LEAST SQUARES FIT,  T=300,2000.
C  PRESS =  1.00
      D 1 1=  1.119300E-04*(T**  1.661400E+00)
      D 1 2=  5.951700E-05*(T**  1.663800E+00)
      D 2 2=  1.537400E-05*(T**  1.672900E+00)
C  SPACE DERIVATIVES.
      YS=Y 3
      X 1=Y 1/YS
      X 2=Y 2/YS
      U 1=U( 1)
      DU 1=UPH( 1)
      DDU 1=UPH2( 1)
      U 2=1.0-U 1
      DU 2=-DU 1
      DDU 2=-DDU 1
      DY 1=DU 1/  2.00
      DY 2=DU 2/ 28.00
      DYS=+DY 1+DY 2
C  TPN =  1.0000E+03      PHN =  5.0000E-05      TMN =  1.0000E-03
      DT=UPH(NPDE)*  1.0000E+03
      DRH=- 1.2187690433E-02*(DT/T+DYS/YS)/(T*YS)
      DYSY=DYS/(YS*YS)
      DX 1=DY 1/YS-Y 1*DYSY
      DL 1=  4.694228307000E-06*(T**( -2.616700E-01))*DT
      RLZ 1=  8.155096200000E-06*(T**(  6.502900E-01))
      DLZ 1=  5.303177507898E-06*(T**( -3.497100E-01))*DT
      DD 1 1=  1.859605020000E-04*(T**(  6.614000E-01))*DT
      VV 1=  4.568922191255E+05*(T**( -6.502900E-01))
      DVV 1= -2.971124411751E+05*(T**( -1.650290E+00))*DT
      XXSV 1=X 1*X 1*VV 1
      DXXSV 1=2.0*X 1*DX 1*VV 1+X 1*X 1*DVV 1
      DX 2=DY 2/YS-Y 2*DYSY
      DL 2=  5.125903692000E-07*(T**( -2.000400E-01))*DT
      RLZ 2=  1.135551728571E-06*(T**(  6.613600E-01))
      DLZ 2=  7.510084912080E-07*(T**( -3.386400E-01))*DT
      DD 2 2=  2.571916460000E-05*(T**(  6.729000E-01))*DT
      VV 2=  2.343731689596E+05*(T**( -6.613600E-01))
      DVV 2= -1.550050390231E+05*(T**( -1.661360E+00))*DT
      XXSV 2=X 2*X 2*VV 2
      DXXSV 2=2.0*X 2*DX 2*VV 2+X 2*X 2*DVV 2
      VD 1 2=  1.680192213989E+04*(T**( -1.663800E+00))
      DVD 1 2= -2.795503805635E+04*(T**( -2.663800E+00))*DT
      XXSD 1 2=X 1*X 2*VD 1 2
      DXXSD 1 2=DX 1*X 2*VD 1 2+X 1*DX 2*VD 1 2+X 1*X 2*DVD 1 2
      XXTSD 1 2=XXSD 1 2*T
      DXTSD 1 2=DXXSD 1 2*T+XXSD 1 2*DT
C  SPECIFIC HEAT OF THE MIXTURE.  NTIS FORMULA.
      CM(IC)=+C(IST+ 1)*U 1+C(IST+ 2)*U 2
C  THERMAL CONDUCTIVITY OF THE MIXTURE.
```

```
C     HIRSHFELDER METHOD FOR MONATOMICS.
C     P. 37A, TOULOUKIEN, LILEY, AND SAXENA.
C     NOTE IN THE FORMULA, LAMBDA MUST BE IN THE SAME UNITS AS D*P/T.
C     LAMBDA=15*R*VISC/(4*M), WHERE R=82.05 CM**3-ATM/MOLE-K.
C     TO CONVERT LAMBDA BACK TO CAL/CM-SEC-K, MULTIPLY BY 1.9872/82.05.
      TASTLJ=T**(  9.055700E-03)
      TBSTLJ=T**( -1.022500E-02)
      DTAST=  9.055700E-03*DT*T**( -9.909443E-01)
      DTBST= -1.022500E-02*DT*T**( -1.010225E+00)
      CNST=  5.475555555556E-01-  1.407397773742E-01*
     * TBSTLJ-  1.670532689818E-01*TASTLJ
      DCNST=-  1.407397773742E-01*DTBST-  1.670532689818E-01*DTAST
      Z( 1, 2)=CNST*XXTSD 1 2
      DZ 1S 2=CNST*DXTSD 1 2+DCNST*XXTSD 1 2
      Z( 2, 1)=Z( 1, 2)
      DZ 2S 1=DZ 1S 2
      CNST=-  3.505777777778E+00+  1.970356883238E+00*
     * TBSTLJ-  1.670532689818E-01*TASTLJ
      DCNST=  1.970356883238E+00*DTBST-  1.670532689818E-01*DTAST
      T 2=-XXTSD 1 2*CNST
      DT 2=-DXTSD 1 2*CNST-XXTSD 1 2*DCNST
      Z( 1, 1)= -2.600040625635E-02*XXSV 1-
     * ( +T 2)
      DZ 1S 1= -2.600040625635E-02*DXXSV 1-
     * ( +DT 2)
      CNST=-  4.199111111111E+00+  1.005284124101E-02*
     * TBSTLJ-  1.670532689818E-01*TASTLJ
      DCNST=  1.005284124101E-02*DTBST-  1.670532689818E-01*DTAST
      T 1=-XXTSD 1 2*CNST
      DT 1=-DXTSD 1 2*CNST-XXTSD 1 2*DCNST
      Z( 2, 2)= -3.640056875889E-01*XXSV 2-
     * ( +T 1)
      DZ 2S 2= -3.640056875889E-01*DXXSV 2-
     * ( +DT 1)
      V( 1)=X 1
      V( 2)=X 2
      CALL DEC( 2,20,Z,IPS,IER)
      CALL SDL( 2,20,Z,V,IPS)
      RLM= -9.687751E-02*( +X 1*V( 1) +X 2*V( 2))
      DV( 1)=DX 1-DZ 1S 1*V( 1)-DZ 1S 2*V( 2)
      DV( 2)=DX 2-DZ 2S 1*V( 1)-DZ 2S 2*V( 2)
      CALL SDL( 2,20,Z,DV,IPS)
      DRLM= -9.687751E-02*( +X 1*DV( 1)+DX 1*V( 1) +
     * X 2*DV( 2)+DX 2*V( 2))
      SUM=+X 2*VD 1 2
      DSUM=+DX 2*VD 1 2+X 2*DVD 1 2
      B=1.0+D 1 1*SUM/X 1
      DB=DD 1 1*SUM/X 1+D 1 1*DSUM/X 1-D 1 1*SUM*DX 1/(X 1*X 1)
      RLM=RLM+(RL 1-RLZ 1)/B
      DRLM=DRLM+(DL 1-DLZ 1)/B-(RL 1-RLZ 1)*DB/(B*B)
      SUM=+X 1*VD 1 2+X 3*VD 2 3
      DSUM=+DX 1*VD 1 2+X 1*DVD 1 2+DX 3*VD 2 3+X 3*DVD 2 3
      B=1.0+D 2 2*SUM/X 2
      DB=DD 2 2*SUM/X 2+D 2 2*DSUM/X 2-D 2 2*SUM*DX 2/(X 2*X 2)
      RLM=RLM+(RL 2-RLZ 2)/B
      DRLM=DRLM+(DL 2-DLZ 2)/B-(RL 2-RLZ 2)*DB/(B*B)
      SUM=+X 1*VD 1 2
```

```
      DSUM=+DX 1*VD 1 2+X 1*DVD 1 2
      B=1.0+D 2 2*SUM/X 2
      DB=DD 2 2*SUM/X 2+D 2 2*DSUM/X 2-D 2 2*SUM*DX 2/(X 2*X 2)
      RLM=RLM+(RL 2-RLZ 2)/B
      DRLM=DRLM+(DL 2-DLZ 2)/B-(RL 2-RLZ 2)*DB/(B*B)
      RHLM(IC)=RH*RLM
      DRHLM(IC)=RH*DRLM+DRH*RLM
C  SOLVE FOR UV.
      V( 2)=0.0
      V( 1)=DX 1*RH/  5.0000E-05
      Z( 2, 1)=U 1
      DZ 2S 1=DU 1
      Z( 2, 2)=U 2
      DZ 2S 2=DU 2
      Z( 1, 2)=XXSD 1 2
      DZ 1S 2=DXXSD 1 2
      Z( 1, 1)=-XXSD 1 2
      DZ 1S 1=-DXXSD 1 2
      Z( 2, 2)=-XXSD 1 2-XXSD 2 3
      DZ 2S 2=-DXXSD 1 2-DXXSD 2 3
      CALL DEC( 2,20,Z,IPS,IER)
      CALL SOL( 2,20,Z,V,IPS)
      UV 1=U 1*V( 1)
      UV 2=U 2*V( 2)
      RHUV(IST+ 1)=RH*UV 1
      RHUV(IST+ 2)=RH*UV 2
C  SPACE DER OF DENSITY TIMES UV.
      DDY 1=DDU 1/  2.00
      DDY 2=DDU 2/ 28.00
      DDYS=+DDY 1+DDY 2
      DYSYSQ=(DYS/YS)**2
      DDX 1=(DDY 1-2.0*DY 1*DYS/YS+2.0*Y 1*DYSYSQ-Y 1*DDYS/YS)/YS
      DDX 2=(DDY 2-2.0*DY 2*DYS/YS+2.0*Y 2*DYSYSQ-Y 2*DDYS/YS)/YS
      DV( 1)=(RH*DDX 1+DRH*DX 1)/  5.0000E-05-DZ 1S 1*V( 1)-
     * DZ 1S 2*V( 2)
      DV( 2)=-DZ 2S 1*V( 1)-DZ 2S 2*V( 2)
      CALL SOL( 2,20,Z,DV,IPS)
      DUV 1=U 1*DV( 1)+DU 1*V( 1)
      DUV 2=U 2*DV( 2)+DU 2*V( 2)
      DRHUV(IST+ 1)=DRH*UV 1+RH*DUV 1
      DRHUV(IST+ 2)=DRH*UV 2+RH*DUV 2
C  FIND THE TIME DERIVATIVES.
      SP=ASP+BSP*TIME
  100 CONTINUE
      IF(KPDE.EQ.NPDE)GO TO 150
      RY=    1.0000000000E-03*R(KPDE)
      DY=-    2.0000000000E+01*DRHUV(IST+KPDE)
      FVAL=SP*UPH(KPDE)+DY+RY
      RETURN
  150 CONTINUE
      TL=    4.0000000000E+05*
     * (DRHLM(IC)*UPH(NPDE)+RHLM(IC)*UPH2(NPDE))
      TD=-    2.0000000000E+01*UPH(NPDE)*( +C(IST+ 1)*RHUV(IST+ 1) +
     * C(IST+ 2)*RHUV(IST+ 2))
      TR=-    1.0000000000E-06*( +P( 1)*H(IST+ 1) +R( 2)*H(IST+ 2))
      FVAL=SP*UPH(NPDE)+(TL+TR+TD)/CM(IC)
      RETURN
```

```
      END                                                            F         230
```

```
      PROGRAM LOADF(INPUT,OUTPUT,TAPE5=INPUT,TAPE6=OUTPUT,
     * TAPE3,TAPE9,TAPE15)
C  LOADF CREATES THE SUBROUTINE F IN FLSC.
      DIMENSION II(72)
      DIMENSION III(44)
      DIMENSION LB(25),W(25),AU(7,25),AL(7,25)
      DIMENSION ALD(25),BLD(25),ABD(25,25),BBD(25,25)
      DIMENSION AV(25),BV(25)
      DIMENSION LBPR(25)
      WRITE(3,1000)
1000  FORMAT(1HC,2X,63HFOR THE COMPLETE TRANSPORT CASE, WE DO NOT WANT T
     *HE U VALUES OR)
      WRITE(3,1005)
1005  FORMAT(1HC,2X,62HTHEIR FIRST DERIVATIVES TO BE ZERO.  THIS CAN LEA
     *D TO DIVISION)
      WRITE(3,1010)
1010  FORMAT(1HC,2X,8HBY ZERO.)
      WRITE(3,1012)
1012  FORMAT(6X,14HDO 5 K=1,NPDEM)
      WRITE(3,1014)
1014  FORMAT(6X,32HIF(ABS(U(K)).LT.SMALL)U(K)=SMALL)
      WRITE(3,1016)
1016  FORMAT(1X,1H5,4X,36HIF(ABS(UPH(K)).LT.SMALL)UPH(K)=SMALL)
      READ(5,12)NLINE
12    FORMAT(10I4)
C  NLINE IS THE NUMBER OF COMMENT LINES TO BE READ AND PRINTED.
      DO 20 K=1,NLINE
      READ(5,22)II
      WRITE(3,22)II
20    CONTINUE
22    FORMAT(72A1)
24    FORMAT(/1X,72A1/)
      READ(5,12)NSPC
      NM=NSPC-1
      LBM=1H-
      LBU=2HU(
      LBP=1H)
      WRITE(3,1020)((LBM,LBU,K,LBP),K=1,NM)
1020  FORMAT(6X,6HYN=1.0,8(A1,A2,I2,A1),A1,2(/5X,1H*,1X,
     *  8(A2,I2,A1,A1))  )
      WRITE(3,1025)
1025  FORMAT(6X,33HCALL RT(U,YN,R,NPDE,KPDE,IC,KSKR) )
      WRITE(3,18)NSPC
18    FORMAT(6X,4H1ST=,I2,7H*(IC-1) )
      DO 30 K=1,NSPC
      READ(5,32)LB(K),W(K)
      WRITE(6,34)K,LB(K),W(K)
      READ(15,36)(AU(L,K),L=1,5),(III(L),L=1,5)
      WRITE(6,36)(AU(L,K),L=1,5),(III(L),L=1,5)
      READ(15,36)(AU(L,K),L=6,7),(AL(L,K),L=1,3),(III(L),L=1,5)
      WRITE(6,36)(AU(L,K),L=6,7),(AL(L,K),L=1,3),(III(L),L=1,5)
      READ(15,37)(AL(L,K),L=4,7),(III(L),L=1,20)
      WRITE(6,37)(AL(L,K),L=4,7),(III(L),L=1,20)
30    CONTINUE
32    FORMAT(A5,7F7.0)
34    FORMAT(/2X,I4,4X,A5,4X,F8.2/)
36    FORMAT(5E15.8,5A1)
```

```
 37   FORMAT(4E15.8,20A1)
      READ(5,232)TPN,PHN,TMN
 232  FORMAT(1P3E12.4)
      WRITE(3,27)
 27   FORMAT(6X,22HIF(KSKT.GT.1)GO TO 100)
      WRITE(3,28)
 28   FORMAT(6X,22HIF(KSKR.GT.1)GO TO 125  )
      READ(5,12)NLINE
      DO 40 K=1,NLINE
      READ(5,22)II
      WRITE(3,22)II
 40   CONTINUE
C  ************************
C  ENTHALPIES AND HEAT CAPACITIES.
C  ************************
      WRITE(3,42)
 42   FORMAT(6X,24HIF(T.GT.1000.)GO TO 2000)
      DO 50 K=1,NSPC
      WRITE(3,52)K,AL(1,K),AL(2,K)
      WRITE(3,54)(AL(L,K),L=3,5)
      WRITE(3,62)K,AL(6,K),AL(1,K)
      WRITE(3,64)AL(2,K),AL(3,K)
      WRITE(3,66)AL(4,K),AL(5,K)
 50   CONTINUE
 52   FORMAT(6X,1HC,I2,9H=1.9872*(,1PE16.8,4H+T*(,1PE16.8)
 54   FORMAT(5X,1H*,1X,3(4H+T*(,1PE16.8),5H)))))
      WRITE(3,56)
 56   FORMAT(6X,10HGO TO 3000)
      WRITE(3,58)
 58   FORMAT(4H2000,2X,8HCONTINUE)
      DO 60 K=1,NSPC
      WRITE(3,52)K,AU(1,K),AU(2,K)
      WRITE(3,54)(AU(L,K),L=3,5)
      WRITE(3,62)K,AU(6,K),AU(1,K)
      WRITE(3,64)AU(2,K),AU(3,K)
      WRITE(3,66)AU(4,K),AU(5,K)
 60   CONTINUE
 62   FORMAT(6X,1HH,I2,9H=1.9872*(,1PE16.8,4H+T*(,1PE16.8)
 64   FORMAT(5X,1H*,1X,4H+T*(,1PE16.8,4H/2.0,4H+T*(,1PE16.8,4H/3.0)
 66   FORMAT(5X,1H*,1X,4H+T*(,1PE16.8,4H/4.0,4H+T*(,1PE16.8,
     * 4H/5.0,6H))))))
      WRITE(3,68)
 68   FORMAT(4H3000,2X,8HCONTINUE)
      WRITE(3,134)
 134  FORMAT(1HC,2X,39HSPECIFIC HEATS AND SPECIFIC ENTHALPIES.  )
      DO 140 K=1,NSPC
      WRITE(3,142)K,K,W(K)
      WRITE(3,144)K,K,W(K)
 140  CONTINUE
 142  FORMAT(6X,6HC(IST+,I2,3H)=C,I2,1H/,F6.2)
 144  FORMAT(6X,6HH(IST+,I2,3H)=H,I2,1H/,F6.2)
      WRITE(3,146)
 146  FORMAT(1X,3H125,2X,8HCONTINUE)
C  ************************
C  THERMAL CONDUCTIVITIES AND BINARY DIFFUSION COEFFICIENTS.
C  READ IN VISCOSITY, THERMAL CONDUCTIVITY, AND BINARY DIFFUSION
C  COEFFICIENTS FROM A FILE CREATED BY VALUES, CY=6.
```

```
      C   ************************
            READ(5,12)NLINE
            DO 72 K=I,NLINE
            READ(5,22)II
            WRITE(6,22)II
      72    WRITE(3,22)II
      79    FORMAT(1HC,5X,IHV,I2,IH=,IPEI4.6,5H*(T**,IPE14.6,IH) )
            READ(5,I2)NLINE
            DO 70 K=I,NLINE
            READ(5,22)II
            WRITE(3,22)II
            WRITE(6,22)II
      70    CONTINUE
            DO 80 K=I,NSPC
            READ(9,82)AV(K),BV(K),III
            WRITE(6,84)K,LB(K),AV(K),BV(K),III
            READ(9,82)ALD(K),BLD(K),III
            WRITE(6,84)K,LB(K),ALD(K),BLD(K),III
      80    CONTINUE
      82    FORMAT(IP2EI4.6,44A1)
      84    FORMAT(/2X,I4,4X,A4,4X,IP2EI4.6,44A1/)
            DO 78 K=I,NSPC
            WRITE(3,79)K,AV(K),BV(K)
      78    CONTINUE
            DO 90 K=1,NSPC
            WRITE(3,92)K,ALD(K),BLD(K)
      90    CONTINUE
      92    FORMAT(6X,2HRL,I2,1H=,IPEI4.6,5H*(T**,IPEI4.6,IH))
            READ(5,I2)NLINE
            DO 100 K=1,NLINE
            READ(5,22)II
            WRITE(3,22)II
            WRITE(6,22)II
      I00   CONTINUE
            NM=NSPC-I
            DO 110 I=I,NSPC
            DO 110 J=I,NSPC
            READ(9,82)ABD(I,J),BBD(I,J),III
            WRITE(6,I12)I,J,LB(I),LB(J),ABD(I,J),BBD(I,J),III
      110   CONTINUE
      I12   FORMAT(/2X,I4,4X,I4,4X,A4,4X,A4,4X,1P2E14.6,44AI/)
            READ(5,II4)PRESS
      I14   FORMAT(F6.0)
            WRITE(3,116)PRESS
      116   FORMAT(IHC,2X,7HPRESS =,F6.2)
            DO 120 I=I,NM
            IP=I+1
            DO 120 J=1P,NSPC
            ABD(I,J)=ABD(I,J)/PRESS
            WRITE(3,122)I,J,ABD(I,J),BBD(I,J)
      120   CONTINUE
      122   FORMAT(1HC,5X,IHD,2I2,1H=,IPE14.6,5H*(T**,1PE14.6,1H) )
      C   ************************
      C   SPACE DERIVATIVES.
      C   ************************
            LBPL=1H+
            WRITE(3,14R)
```

```
  148 FORMAT(1HC,2X,18HSPACE DERIVATIVES.)
      NS=NSPC+1
      WRITE(3,149)NS
  149 FORMAT(6X,4HYS=Y,I2)
      DO 150 K=1,NSPC
      WRITE(3,152)K,K
  150 CONTINUE
  152 FORMAT(6X,1HX,I2,2H=Y,I2,3H/YS)
      DO 160 K=1,NM
      WRITE(3,162)K,K
      WRITE(3,164)K,K
      WRITE(3,166)K,K
  160 CONTINUE
  162 FORMAT(6X,1HU,I2,3H=U(,I2,1H))
  164 FORMAT(6X,2HDU,I2,5H=UPH(,I2,1H))
  166 FORMAT(6X,3HDDU,I2,6H=UPH2(,I2,1H))
      LBU=1HU
      WRITE(3,172)NSPC,((LBM,LBU,K),K=1,NM)
  172 FORMAT(6X,1HU,I2,4H=1.0,8(A1,A1,I2),A1,2(/5X,1H*,1X,
     *  8(A1,I2,A1)) )
      LBDU=2HDU
      WRITE(3,174)NSPC,((LBM,LBDU,K),K=1,NM)
  174 FORMAT(6X,2HDU,I2,1H=,8(A1,A2,I2),A1,2(/5X,1H*,1X,
     *  8(A2,I2,A1)) )
      LBDDU=3HDDU
      WRITE(3,176)NSPC,((LBM,LBDDU,K),K=1,NM)
  176 FORMAT(6X,3HDDU,I2,1H=,8(A1,A3,I2),A1,2(/5X,1H*,1X,
     *  8(A3,I2,A1)) )
      DO 180 K=1,NSPC
      WRITE(3,182)K,K,W(K)
  180 CONTINUE
  182 FORMAT(6X,2HDY,I2,3H=DU,I2,1H/,F6.2)
      LBDY=2HDY
      WRITE(3,186)((LBPL,LBDY,K),K=1,NSPC)
  186 FORMAT(6X,4HDYS=,8(A1,A2,I2),A1,2(/5X,1H*,1X,8(A2,I2,A1)) )
      PSR=PRESS/82.05
      WRITE(3,234)TPN,PHN,TMN
      WRITE(6,234)TPN,PHN,TMN
  234 FORMAT(1HC,2X,5HTPN =,1PE12.4,6X,5HPHN =,1PE12.4,6X,
     * 5HTMN =,1PE12.4)
      WRITE(3,226)TPN
  226 FORMAT(6X,13HDT=UPH(NPDE)*,1PE12.4)
      WRITE(3,242)PSR
  242 FORMAT(6X,5HDRH=-,1PE18.10,21H*(DT/T+DYS/YS)/(T*YS))
      DO 815 I=1,NSPC
      DO 815 J=I,NSPC
      IF(I.EQ.J)GO TO 815
      A=1.0/ABD(I,J)
      B=-BBD(I,J)
      WRITE(3,818)I,J,A,B
  815 CONTINUE
  818 FORMAT(6X,2HVD,2I2,1H=,1PE16.8,6H*(T**(,1PE16.8,2H)) )
      DO 820 I=1,NSPC
      DO 820 J=I,NSPC
      IF(I.EQ.J)GO TO 820
      A=1.0/ABD(I,J)
      B=-BBD(I,J)
```

```
          A=A*B
          B=B-I.0
          WRITE(3,822)I,J,A,B
  820     CONTINUE
  822     FORMAT(6X,3HOVD,2I2,1H=,IPEI6.8,6H*(T**(,1PEI6.8,5H))*DT)
C     ************************
C     SPECIFIC HEAT OF THE MIXTURE.
C     ************************
          WRITE(3,I24)
  124     FORMAT(IHC,2X,44HSPECIFIC HEAT OF THE MIXTURE.  NTIS FORMULA. )
          LBC=6HC(IST+
          LBU=3H)*U
          WRITE(3,132)((LBPL,LBC,K,LBU,K),K=I,NSPC)
  I32     FORMAT(6X,7HCM(IC)=,4(AI,A6,I2,A3,I2),AI,
         * 4(/5X,IH*,IX,4(A6,12,A3,I2,AI)) )
C     ************************
C     THERMAL CONDUCTIVITY OF THE MIXTURE.
C     ************************
          WRITE(3,272)
          WRITE(3,274)
  272     FORMAT(1HC,2X,36HTHERMAL CONDUCTIVITY OF THE MIXTURE.)
  274     FORMAT(1HC,2X,24HMASON AND SAXENA METHOD.     )
          WRITE(3,252)
  252     FORMAT(1HC,2X,55HLMIX=SUM(I)(L 1/(I.0+(SUM(J)P I J*X J)/X I))
         *I.NE.J     )
          WRITE(3,254)
  254     FORMAT(IHC,2X,69HP I J=(1.065/SQRT(8.0*(1.0+M I/M J)))*(1.0+SQRT((
         *M J*V I)/(M I*V J))*       )
          WRITE(3,255)
  255     FORMAT(IHC,2X,23HSQRT(SQRT(M I/M J)))**2     )
          WRITE(3,256)
  256     FORMAT(1HC,2X,45HP 1 J IS A FUNCTION OF T AND CONSTANTS.        )
          WRITE(3,258)
  258     FORMAT(IHC,2X,45HFOR CONVENIENCE, P I J = A*(I.0+B*T**C)**2     )
          DO 275 I=I,NSPC
          DO 275 J=I,NSPC
          IF(I.EQ.J)GO TO 275
          A=I.065/(2.0*SQRT(2.0*(I.0+W(I)/W(J))))
          B=SQRT(AV(I)/AV(J))*SQRT(SQRT(W(J)/W(I)))
          C=(BV(I)-BV(J))/2.0
          WRITE(3,271)B,C
  27I     FORMAT(6X,8HBTC=I.0+,1PE20.I0,5H*T**(,1PE20.I0,IH) )
          WRITE(3,278)I,J,A
          D=2.0*A*B*C
          E=C-I.0
          WRITE(3,279)I,J,D,E
  275     CONTINUE
  278     FORMAT(6X,1HP,I2,IHS,I2,1H=,IPE20.I0,7H*BTC**2)
  279     FORMAT(6X,2HDP,I2,IHS,I2,1H=,1PE20.10,5H*T**(,1PE20.I0,8H)*BTC*DT)
          LBPS=1HP
          LBX=2H*X
          LBSP=1HS
          K=1
          WRITE(3,282)K,((LBPL,LBPS,K,LBSP,J,LBX,J),J=2,NSPC)
  282     FORMAT(6X,4HSUMP,I2,1H=,5(2A1,I2,AI,12,A2,12),AI,
         * 3(/5X,1H*,1X,5(AI,12,A1,12,A2,I2,AI)) )
          IF(NM.EQ.1)GO TO 284
```

```
      DO 280 K=2,NM                                                    MAIN     286
      KM=K-1                                                           MAIN     287
      KP=K+1                                                           MAIN     288
      WRITE(3,282)K,((LBPL,LBPS,K,LBSP,J,LBX,J),J=1,KM),               MAIN     289
     * ((LBPL,LBPS,K,LBSP,J,LBX,J),J=KP,NSPC)                          MAIN     290
  280 CONTINUE                                                         MAIN     291
  284 CONTINUE                                                         LOADS      2
      K=NSPC                                                           MAIN     292
      WRITE(3,282)K,((LBPL,LBPS,K,LBSP,J,LBX,J),J=1,NM)                MAIN     293
      DO 285 K=1,NSPC                                                  MAIN     294
      WRITE(3,288)K,K,K                                                MAIN     295
  285 CONTINUE                                                         MAIN     296
  288 FORMAT(6X,1HB,I2,9H=1.0+SUMP,I2,2H/X,I2)                         MAIN     297
      LBRL=2HRL                                                        MAIN     298
      LBSB=2H/B                                                        MAIN     299
      WRITE(3,292)((LBPL,LBRL,K,LBSB,K),K=1,NSPC)                      MAIN     300
  292 FORMAT(6X,4HRLM=,6(A1,A2,I2,A2,I2),A1,3(/5X,1H*,1X,              MAIN     301
     * 6(A2,I2,A2,I2,A1)) )                                            MAIN     302
      WRITE(3,306)                                                     MAIN     303
  306 FORMAT(6X,15HRHLM(IC)=RH*RLM)                                    MAIN     304
C     ************************                                         MAIN     305
C     DERIVATIVE OF THE THERMAL CONDUCTIVITY OF THE MIXTURE.           MAIN     306
C     ************************                                         MAIN     307
      WRITE(3,312)                                                     MAIN     308
  312 FORMAT(1HC,2X,40HSPACE DER OF DENSITY TIMES THERMAL COND.)       MAIN     309
      DO 740 K=1,NSPC                                                  MAIN     310
      A=ALD(K)*BLD(K)                                                  MAIN     311
      B=BLD(K)-1.0                                                     MAIN     312
      WRITE(3,742)K,A,B                                                MAIN     313
  740 CONTINUE                                                         MAIN     314
  742 FORMAT(6X,3HDRL,I2,1H=,1PE14.6,6H*(T**(,1PE14.6,5H))*DT   )      MAIN     315
      WRITE(3,745)                                                     MAIN     316
  745 FORMAT(6X,16HDYSY=DYS/(YS*YS)  )                                 MAIN     317
      DO 750 K=1,NSPC                                                  MAIN     318
      WRITE(3,752)K,K,K                                                MAIN     319
  750 CONTINUE                                                         MAIN     320
  752 FORMAT(6X,2HDX,I2,3H=DY,I2,5H/YS-Y,I2,5H*DYSY  )                 MAIN     321
      LBX=2H*X                                                         MAIN     322
      LBDX=3H*DX                                                       MAIN     323
      LBPS=1HP                                                         MAIN     324
      LBDP=2HDP                                                        MAIN     325
      K=1                                                              MAIN     326
      WRITE(3,762)K,((LBPL,LBDP,K,LBSP,J,LBX,J,LBPL,LBPS,K,LBSP,J,     MAIN     327
     * LBDX,J),J=2,NSPC)                                               MAIN     328
      IF(NM.EQ.1)GO TO 761                                             LOADS      3
      DO 760 K=2,NM                                                    MAIN     329
      KM=K-1                                                           MAIN     330
      KP=K+1                                                           MAIN     331
      WRITE(3,762)K,((LBPL,LBDP,K,LBSP,J,LBX,J,LBPL,LBPS,K,LBSP,J,LBDX, MAIN    332
     * J),J=1,KM),((LBPL,LBDP,K,LBSP,J,LBX,J,LBPL,LBPS,K,LBSP,J,LBDX,J), MAIN   333
     * J=KP,NM)                                                        MAIN     334
  760 CONTINUE                                                         MAIN     335
  761 CONTINUE                                                         LOADS      4
      K=NSPC                                                           MAIN     336
      WRITE(3,762)K,((LBPL,LBDP,K,LBSP,J,LBX,J,LBPL,LBPS,K,LBSP,       MAIN     337
     * J,LBDX,J),J=1,NM)                                               MAIN     338
  762 FORMAT(6X,5HDSUMP,I2,1H=,2(A1,A2,I2,A1,I2,A2,I2,2A1,I2,A1,I2,A3, MAIN     339
```

```
      * I2),A1,9(/5X,1H*,1X,2(A2,I2,A1,I2,A2,I2,2A1,I2,A1,I2,A3,I2,A1)) ) MAIN  340
        DO 765 K=I,NSPC                                                    MAIN  341
        WRITE(3,768)K,K,K,K,K,K                                            MAIN  342
  765   CONTINUE                                                           MAIN  343
  768   FORMAT(6X,2HDB,I2,1H=,6H(DSUMP,I2,5H-SUMP,I2,3H*OX,I2,2H/X,I2,     MAIN  344
      * 3H)/X,I2)                                                          MAIN  345
        DO 770 K=I,NSPC                                                    MAIN  346
        WRITE(3,772)K,K,K,K,K,K                                            MAIN  347
  770   CONTINUE                                                           MAIN  348
  772   FORMAT(6X,1HT,I2,5H=(ORL,I2,3H-RL,I2,3H*OB,I2,2H/B,I2,3H)/B,I2)    MAIN  349
        LBT=IHT                                                            MAIN  350
        WRITE(3,776)((LBPL,LBT,K),K=I,NSPC)                                MAIN  351
  776   FORMAT(6X,5HORLM=,I0(2A1,I2),AI,/5X,1H*,IX,I0(AI,I2,AI)  )         MAIN  352
        WRITE(3,778)                                                       MAIN  353
  778   FORMAT(6X,25HDRHLM(IC)=ORH*RLM+RH*DRLM)                            MAIN  354
C    *************************                                             MAIN  355
C    SOLVE FOR UV.                                                         MAIN  356
C    ZERO ORDER BORIS AND ORAN APPROXIMATION.                              MAIN  357
C    *************************                                             MAIN  358
        WRITE(3,400)                                                       MAIN  359
  400   FORMAT(1HC,2X,I3HSOLVE FOR UV.)                                    MAIN  360
        LBX=IHX                                                            MAIN  361
        LBVD=3H*VD                                                         MAIN  362
        K=I                                                                MAIN  363
        WRITE(3,402)K,((LBPL,LBX,J,LBVD,K,J),J=2,NSPC)                     MAIN  364
  402   FORMAT(6X,3HSUM,I2,1H=,5(2A1,I2,A3,2I2),AI,3(/5X,IH*,IX,           MAIN  365
      * 5(AI,I2,A3,2I2,AI)) )                                              MAIN  366
        IF(NM.EQ.1)GO TO 412                                               LOA05   5
        DO 410 K=2,NM                                                      MAIN  367
        KM=K-I                                                             MAIN  368
        KP=K+1                                                             MAIN  369
        WRITE(3,402)K,((LBPL,LBX,J,LBVD,J,K),J=I,KM),((LBPL,LBX,J,         MAIN  370
      * LBVD,K,J),J=KP,NSPC)                                               MAIN  371
  410   CONTINUE                                                           MAIN  372
  412   CONTINUE                                                           LOA05   6
        K=NSPC                                                             MAIN  373
        WRITE(3,402)K,((LBPL,LBX,J,LBVD,J,K),J=1,NM)                       MAIN  374
        DO 415 K=I,NSPC                                                    MAIN  375
        WRITE(3,418)K,K,K,PHN                                              MAIN  376
  415   CONTINUE                                                           MAIN  377
  418   FORMAT(6X,1HB,I2,2H=X,I2,4H*SUM,I2,1H*,1PE12.4)                    MAIN  378
        DO 420 K=I,NSPC                                                    MAIN  379
        WRITE(3,422)K,K                                                    MAIN  380
  420   CONTINUE                                                           MAIN  381
  422   FORMAT(6X,1HT,I2,11H=-RH*(1.0-U,I2,1H) )                           MAIN  382
        DO 425 K=I,NSPC                                                    MAIN  383
        WRITE(3,428)K,K,K                                                  MAIN  384
  425   CONTINUE                                                           MAIN  385
  428   FORMAT(6X,3HFAC,I2,2H=T,I2,2H/B,I2)                                MAIN  386
        DO 465 K=I,NSPC                                                    MAIN  387
        WRITE(3,468)K,K,K                                                  MAIN  388
  465   CONTINUE                                                           MAIN  389
  468   FORMAT(6X,1HV,I2,4H=FAC,I2,3H*DX,I2)                               MAIN  390
        DO 470 K=I,NSPC                                                    MAIN  391
        WRITE(3,472)K,K,K                                                  MAIN  392
  470   CONTINUE                                                           MAIN  393
  472   FORMAT(6X,2HUV,I2,2H=U,I2,2H*V,I2)                                 MAIN  394
```

```
          LBUV=2HUV                                                        MAIN    395
          WRITE(3,476)((LBM,LBUV,K),K=1,NSPC)                              MAIN    396
      476 FORMAT(6X,3HDV=,8(A1,A2,I2),A1,2(/5X,1H*,1X,8(A2,I2,A1)) )       MAIN    397
          DO 480 K=1,NSPC                                                  MAIN    398
          WRITE(3,482)K,K,K                                                MAIN    399
      480 CONTINUE                                                         MAIN    400
      482 FORMAT(6X,2HUV,I2,3H=UV,I2,5H*DV*U,I2)                           MAIN    401
          DO 485 K=1,NSPC                                                  MAIN    402
          WRITE(3,488)K,K                                                  MAIN    403
      485 CONTINUE                                                         MAIN    404
      488 FORMAT(6X,9HRHUV(1ST+,I2,7H)=RH*UV,I2)                           MAIN    405
      C  ************************                                          MAIN    406
      C  SOLVE FOR THE SPACE DERIVATIVE OF UV.                             MAIN    407
      C  ************************                                          MAIN    408
          WRITE(3,522)                                                     MAIN    409
      522 FORMAT(1HC,2X,30HSPACE DER OF DENSITY TIMES UV.)                 MAIN    410
          DO 500 K=1,NSPC                                                  MAIN    411
          WRITE(3,502)K,K,W(K)                                             MAIN    412
      500 CONTINUE                                                         MAIN    413
      502 FORMAT(6X,3HDDY,I2,4H=DDU,I2,1H/,F6.2)                           MAIN    414
          LBDDY=3HDDY                                                      MAIN    415
          WRITE(3,506)((LBPL,LBDDY,K),K=1,NSPC)                            MAIN    416
      506 FORMAT(6X,5HDDYS=,8(A1,A3,I2),A1,2(/5X,1H*,1X,8(A3,I2,A1)) )     MAIN    417
          WRITE(3,510)                                                     MAIN    418
      510 FORMAT(6X,18HDYSYSQ=(DYS/YS)**2 )                                MAIN    419
          DO 515 K=1,NSPC                                                  MAIN    420
          WRITE(3,518)K,K,K,K,K                                            MAIN    421
      515 CONTINUE                                                         MAIN    422
      518 FORMAT(6X,3HDDX,I2,5H=(DDY,I2,7H-2.0*DY,I2,13H*DYS/YS+2.0*Y,     MAIN    423
         * I2,9H*DYSYSQ-Y,I2,12H*DDYS/YS)/YS  )                            MAIN    424
          LBDX=2HDX                                                        MAIN    425
          LBVD=3H*VD                                                       MAIN    426
          LBX=1HX                                                          MAIN    427
          LBDVD=4H*DVD                                                     MAIN    428
          K=1                                                              MAIN    429
          WRITE(3,532)K,((LBPL,LBDX,J,LBVD,K,J,LBPL,LBX,J,LBDVD,K,J),      MAIN    430
         * J=2,NSPC)                                                       MAIN    431
      532 FORMAT(6X,4HDSUM,I2,1H=,2(A1,A2,I2,A3,2I2,2A1,I2,A4,2I2),A1,     MAIN    432
         * 9(/5X,1H*,1X,2(A2,I2,A3,2I2,2A1,I2,A4,2I2,A1)) )                MAIN    433
          IF(NM.EQ.1)GO TO 541                                             LOAD5     7
          DO 535 K=2,NM                                                    MAIN    434
          KM=K-I                                                           MAIN    435
          KP=K+1                                                           MAIN    436
          WRITE(3,532)K,((LBPL,LBDX,J,LBVD,J,K,LBPL,LBX,J,LBDVD,J,K),      MAIN    437
         * J=1,KM),((LBPL,LBDX,J,LBVD,K,J,LBPL,LBX,J,LBDVD,K,J),J=KP,NSPC) MAIN    438
      535 CONTINUE                                                         MAIN    439
          K=NSPC                                                           MAIN    440
          WRITE(3,532)K,((LBPL,LBDX,J,LBVD,J,K,LBPL,LBX,J,LBDVD,J,K),J=1,NM) MAIN  441
          DO 540 K=I,NSPC                                                  MAIN    442
          WRITE(3,542)K,PHN,K,K,K,K                                        MAIN    443
      540 CONTINUE                                                         MAIN    444
      541 CONTINUE                                                         LOAD5     8
      542 FORMAT(6X,2HDB,I2,1H=,1PE12.4,4H*(DX,I2,4H*SUM,I2,2H+X,I2,       MAIN    445
         * 5H*DSUM,I2,IH) )                                                MAIN    446
          DO 545 K=1,NSPC                                                  MAIN    447
          WRITE(3,548)K,K,K                                                MAIN    448
      545 CONTINUE                                                         MAIN    449
```

```
548   FORMAT(6X,2HDT,I2,12H=-DRH*(1.0-U,I2,7H) +RH*DU,I2)
      DO 550 K=1,NSPC
      WRITE(3,552)(K,L=I,7)
550   CONTINUE
552   FORMAT(6X,4HDFAC,I2,1H=,2HDT,I2,2H/B,I2,2H-T,12,3H*DB,I2,
     * 3H/(B,I2,2H*B,12,1H) )
      DO 590 K=1,NSPC
      WRITE(3,592)K,K,K,K,K
590   CONTINUE
592   FORMAT(6X,2HDV,I2,5H=DFAC,I2,3H*DX,I2,4H+FAC,I2,4H*DDX,I2)
      DO 595 K=1,NSPC
      WRITE(3,598)K,K,K,K,K
595   CONTINUE
598   FORMAT(6X,3HDUV,I2,3H=DU,I2,2H*V,I2,2H+U,I2,3H*DV,I2)
      LBDUV=3HDUV
      WRITE(3,802)((LBM,LBDUV,K),K=1,NSPC)
802   FORMAT(6X,4HDDV=,8(A1,A3,I2),A1,2(/5X,IH*,IX,8(A3,I2,AI)) )
      DO 805 K=I,NSPC
      WRITE(3,808)K,K,K,K
805   CONTINUE
808   FORMAT(6X,3HDUV,I2,4H=DUV,I2,6H+DV*DU,I2,6H+DDV*U,I2)
      DO 8I0 K=1,NSPC
      WRITE(3,8I2)K,K,K
8I0   CONTINUE
8I2   FORMAT(6X,IOHDRHUV(IST+,I2,8H)=DRH*UV,I2,7H+RH*DUV,I2)
C   ***********************
C   FIND THE TIME DERIVATIVES.
C   ***********************
      WRITE(3,6I2)
6I2   FORMAT(IHC,2X,26HFIND THE TIME DERIVATIVES.)
      WRITE(3,622)
622   FORMAT(6X,I5HSP=ASP+BSP*TIME)
      TMSPH2=TMN/(PHN*PHN)
      WRITE(3,628)
628   FORMAT(1X,3H100,2X,8HCONTINUE)
      WRITE(3,632)
632   FORMAT(6X,25HIF(KPDE.EQ.NPDE)GO TO 150)
      WRITE(3,636)TMN
636   FORMAT(6X,3HRY=,IPE20.10,8H*R(KPDE) )
      TMSPH=TMN/PHN
      WRITE(3,638)TMSPH
638   FORMAT(6X,4HDY=-,IPE20.10,I6H*DRHUV(IST+KPDE) )
      WRITE(3,642)
642   FORMAT(6X,23HFVAL=SP*UPH(KPDE)+DY+RY)
      WRITE(3,646)
646   FORMAT(6X,6HRETURN)
      WRITE(3,648)
648   FORMAT(IX,3H150,2X,8HCONTINUE)
      DO 650 K=I,NM
      WRITE(3,652)K,K
650   CONTINUE
652   FORMAT(6X,2HDU,12,5H=UPH(,I2,1H) )
      K=NSPC
      LBDU=2HDU
      WRITE(3,656)K,((LBM,LBDU,J),J=I,NM)
656   FORMAT(6X,2HDU,I2,IH=,8(A1,A2,12),A1,2(/5X,1H*,IX,8(A2,12,AI)) )
      WRITE(3,662)TMSPH2
```

```
  662   FORMAT(6X,3HTL=,1PE20.10,1H*)
        WRITE(3,664)
  664   FORMAT(5X,1H*,1X,41H(DRHLM(IC)*UPH(NPDE)+RHLM(IC)*UPH2(NPDE)) )
        LBBL=1H
        LBC=6HC(1ST+
        LBRHUV=10H)*RHUV(IST
        WRITE(3,668)TMSPH,((LBBL,LBPL,LHC,K,LBRHUV,LBPL,K,LBP),K=1,
       * NSPC),LBP
  668   FORMAT(6X,4HTD=-,1PE20.10,12H*UPH(NPDE)*(,2A1,A6,I2,A10,A1,I2,
       * 3A1,10(/5X,1H*,1X,2(A6,I2,A10,A1,I2,3A1)) )
        TMSTP=TMN/TPN
        LBR=2HR(
        LBH=8H)*H(1ST+
        WRITE(3,672)TMSTP,((LBBL,LBPL,LHR,K,LBH,K,LBP),K=1,NSPC),LBP
  672   FORMAT(6X,4HTR=-,1PE20.10,2H*(,2(2A1,A2,I2,A8,I2,A1),2A1,
       * 9(/5X,1H*,1X,2(A2,I2,A8,I2,3A1)) )
        WRITE(3,676)
  676   FORMAT(6X,35HFVAL=SP*UPH(NPDE)+(TL+TR+TD)/CM(IC) )
        STOP
        END
```

```
        S C O P E   2   L O A D   M A P                                   LOADER VERSION 1.0    04/15/80  14.46.14.  PAGE    1
PROGRAM  WILL BE ENTERED AT  LOADF      (    241)                         SCM LENGTH     16152           LCM LENGTH          0

        BLOCK          ADDRESS    LENGTH      FILE

        LOADF            110      11104        LGO
         /STP.END/     11214          1      SL-FTNLIB
         /FCL.C./      11215         30      SL-FTNLIB
         /Q8.10./      11245        144      SL-FTNLIB
        Q2NTRY=        11411          4      SL-FTNLIB
        COMIO=         11415         10      SL-FTNLIB
        FECMSK=        11425         41      SL-FTNLIB
        FEIFST=        11466          3      SL-FTNLIB
        FLTIN=         11471        156      SL-FTNLIB
        FLTOUT=        11647        315      SL-FTNLIB
        FMTAP=         12164        377      SL-FTNLIB
        FORSYS=        12563        300      SL-FTNLIB
        FORUTL=        13063         45      SL-FTNLIB
        GETFIT=        13130         54      SL-FTNLIB
        INCOM=         13204        144      SL-FTNLIB
        INPC=          13350        173      SL-FTNLIB
        KOOER=         13543        476      SL-FTNLIB
        KRAKER=        14241        454      SL-FTNLIB
        OUTC=          14715        155      SL-FTNLIB
        OUTCOM=        15072        204      SL-FTNLIB
        ERRCAP=        15276        317      SL-FTNLIB
        FERCAP=        15615        171      SL-FTNLIB
        EXP.MSG        16006         16      SL-FTNLIB
        SQRT           16024          6      SL-FTNLIB
        SQRT.          16032         32      SL-FTNLIB
        SYSAID=        16064          1      SL-FTNLIB
        SYS=1ST        16065         65      SL-FTNLIB

    1   H2             2.00

 .31001901E+01  .51119464E-03  .52644210E-07 -.34909973E-10  .36945345E-14   H2
-.87738042E+03 -.19629421E+01  .30574451E+01  .26765200E-02 -.58099162E-05   H2
 .55210391E-08 -.18122739E-11 -.98890474E+03 -.22997056E+01                  H2

    2   N2            28.00

 .28963194E+01  .15154866E-02 -.57235277E-06  .99807393E-10 -.65223555E-14   N2
-.90586184E+03  .61615148E+01  .36748261E+01 -.12081500E-02  .23240102E-05   N2
-.63217559E-09 -.22577253E-12 -.10611588E+04  .23580424E+01                  N2
  VISCOSITY FROM WARNATZ ST PAR.
  LEAST SQUARES FIT,   T=300,2000.
  THERMAL CONDUCTIVITIES FROM WARNATZ ST PAR.
  LEAST SQUARES FIT,   T=300,2000.

    1   H2          2.188700E-06  6.502900E-01    H2      VISCOSITY.

    1   H2          6.357900E-06  7.383300E-01    H2      THERMAL CONDUCTIVITY.

    2   N2          4.266700E-06  6.613600E-01    N2      VISCOSITY.

    2   N2          6.407700E-07  7.999600E-01    N2      THERMAL CONDUCTIVITY.
```

BINARY DIFFUSION COEFFICIENTS FROM WARNATZ ST PAR.
LEAST SQUARES FIT. T=300.2000.

1	1	H2	H2	1.119300E-04	1.661400E+00	H2	H2	BINARY DIFFUSION.
1	2	H2	N2	5.951700E-05	1.663800E+00	H2	N2	BINARY DIFFUSION.
2	2	N2	N2	1.537400E-05	1.672900E+00	N2	N2	BINARY DIFFUSION.

TPN = 1.0000E+03 PHN = 5.0000E-05 TMN = 1.0000E-03

```
      SUBROUTINE F(TIME,PH,U,UPH,UPH2,FVAL,NPDE,KPDE,IC,KSKT,KSKR)
      DIMENSION U(NPDE),UPH(NPDE),UPH2(NPDE)
      COMMON/TABAB/ASP,BSP,TPN,PHN,TMN,TMSPH,TMSPH2,TMSTP,TPENT
      COMMON/TABP/PRESS,PSR,NPDEM
      COMMON/TABSM/SMALL
      COMMON/TABAM/YAB,WAB
      DIMENSION R(20)
      DIMENSION C(1000),H(1000),RHLM(100),DRHLM(100),CM(100)
      COMMON/TABCT/RL,CPMX,HO(20),R2D(20),R2DM(20)
      COMMON/TABMF/RHUV(1000),DRHUV(1000)
      COMMON/TABRY/T,RH,Y1,Y2,Y3,Y4,Y5,Y6,Y7,Y8,Y9,Y10
C  AT EACH CALL THE TIME RATE OF CHANGE FOR ONE PDE IS RETURNED IN FVAL.
C  FOR THE COMPLETE TRANSPORT CASE, WE DO NOT WANT THE U VALUES OR
C  THEIR FIRST DERIVATIVES TO BE ZERO.  THIS CAN LEAD TO DIVISION
C  BY ZERO.
      DO 5 K=1,NPDEM
      IF(ABS(U(K)).LT.SMALL)U(K)=SMALL
    5 IF(ABS(UPH(K)).LT.SMALL)UPH(K)=SMALL
C  TEST CASE.  BINARY MIX OF H2 AND N2.  TRANSPORT WARNATZ PAR.
C  U = MASS FRACTIONS.  Y = MASS FRACTIONS / MOLECULAR WEIGHTS.
      YN=1.0-U( 1)
      CALL RT(U,YN,R,NPDE,KPDE,IC,KSKR)
      IST= 2*(IC-1)
      IF(KSKT.GT.1)GO TO 100
      IF(KSKR.GT.1)GO TO 125
C  NTIS ENTHALPIES AND HEAT CAPACITIES.
      IF(T.GT.1000.)GO TO 2000
      C 1=1.9872*(  3.05744510E+00+T*(  2.67652000E-03
     * +T*( -5.80991620E-06+T*(  5.52103910E-09+T*( -1.81227390E-12)))))
      H 1=1.9872*( -9.88904740E+02+T*(  3.05744510E+00
     * +T*(  2.67652000E-03/2.0+T*( -5.80991620E-06/3.0
     * +T*(  5.52103910E-09/4.0+T*( -1.81227390E-12/5.0))))))
      C 2=1.9872*(  3.67482610E+00+T*( -1.20815000E-03
     * +T*(  2.32401020E-06+T*( -6.32175590E-10+T*( -2.25772530E-13)))))
      H 2=1.9872*( -1.06115880E+03+T*(  3.67482610E+00
     * +T*( -1.20815000E-03/2.0+T*(  2.32401020E-06/3.0
     * +T*( -6.32175590E-10/4.0+T*( -2.25772530E-13/5.0))))))
      GO TO 3000
 2000 CONTINUE
      C 1=1.9872*(  3.10019010E+00+T*(  5.11194640E-04
     * +T*(  5.26442100E-08+T*( -3.49099730E-11+T*(  3.69453450E-15)))))
      H 1=1.9872*( -8.77380420E+02+T*(  3.10019010E+00
     * +T*(  5.11194640E-04/2.0+T*(  5.26442100E-08/3.0
     * +T*( -3.49099730E-11/4.0+T*(  3.69453450E-15/5.0))))))
      C 2=1.9872*(  2.89631940E+00+T*(  1.51548660E-03
     * +T*( -5.72352770E-07+T*(  9.98073930E-11+T*( -6.52235550E-15)))))
      H 2=1.9872*( -9.05861840E+02+T*(  2.89631940E+00
     * +T*(  1.51548660E-03/2.0+T*( -5.72352770E-07/3.0
     * +T*(  9.98073930E-11/4.0+T*( -6.52235550E-15/5.0))))))
 3000 CONTINUE
C  SPECIFIC HEATS AND SPECIFIC ENTHALPIES.
      C(IST+ 1)=C 1/  2.00
      H(IST+ 1)=H 1/  2.00
      C(IST+ 2)=C 2/ 28.00
      H(IST+ 2)=H 2/ 28.00
  125 CONTINUE
C  VISCOSITY FROM WARNATZ ST PAR.
```

```
C  LEAST SQUARES FIT,  T=300,2000.
C  THERMAL CONDUCTIVITIES FROM WARNATZ ST PAR.
C  LEAST SQUARES FIT,  T=300,2000.
C     V 1=  2.188700E-06*(T**  6.502900E-01)
C     V 2=  4.266700E-06*(T**  6.613600E-01)
      RL 1=  6.357900E-06*(T**  7.383300E-01)
      RL 2=  6.407700E-07*(T**  7.999600E-01)
C  BINARY DIFFUSION COEFFICIENTS FROM WARNATZ ST PAR.
C  LEAST SQUARES FIT,  T=300,2000.
C  PRESS =  1.00
C     D 1 2=  5.951700E-05*(T**  1.663800E+00)
C  SPACE DERIVATIVES.
      YS=Y 3
      X 1=Y 1/YS
      X 2=Y 2/YS
      U 1=U( 1)
      DU 1=UPH( 1)
      DDU 1=UPH2( 1)
      U 2=1.0-U 1
      DU 2=-DU 1
      DDU 2=-DDU 1
      DY 1=DU 1/  2.00
      DY 2=DU 2/ 28.00
      DYS=+DY 1+DY 2
C  TPN =  1.0000E+03      PHN =  5.0000E-05      TMN =  1.0000E-03
      DT=UPH(NPDE)*  1.0000E+03
      DRH=-  1.2187690433E-02*(DT/T+DYS/YS)/(T*YS)
      VD 1 2=  1.68019221E+04*(T**( -1.66380000E+00))
      DVD 1 2= -2.79550381E+04*(T**( -2.66380000E+00))*DT
C  SPECIFIC HEAT OF THE MIXTURE.  NTIS FORMULA.
      CM(IC)=+C(IST+ 1)*U 1+C(IST+ 2)*U 2
C  THERMAL CONDUCTIVITY OF THE MIXTURE.
C  MASON AND SAXENA METHOD.
C  LMIX=SUM(I)(L I/(1.0+(SUM(J)P I J*X J)/X I))       I.NE.J
C  P I J=(1.065/SQRT(8.0*(1.0+M I/M J)))*(1.0+SQRT((M J*V I)/(M I*V J))*
C  SQRT(SQRT(M I/M J)))**2
C  P I J IS A FUNCTION OF T AND CONSTANTS.
C  FOR CONVENIENCE, P I J = A*(1.0+B*T**C)**2
      BTC=1.0+     1.3854124113E+00*T**(    -5.5350000000E-03)
      P 1S 2=     3.6376675219E-01*BTC**2
      DP 1S 2=     -5.5789143943E-03*T**(    -1.0055350000E+00)*BTC*DT
      BTC=1.0+     7.2180672836E-01*T**(     5.5350000000E-03)
      P 2S 1=     9.7220753957E-02*BTC**2
      DP 2S 1=     7.7683275937E-04*T**(    -9.9446500000E-01)*BTC*DT
      SUMP 1=+P 1S 2*X 2
      SUMP 2=+P 2S 1*X 1
      B 1=1.0+SUMP 1/X 1
      B 2=1.0+SUMP 2/X 2
      RLM=+RL 1/B 1+RL 2/B 2
      RHLM(IC)=RH*RLM
C  SPACE DER OF DENSITY TIMES THERMAL COND.
      DRL 1=  4.694228E-06*(T**( -2.616700E-01))*DT
      DRL 2=  5.125904E-07*(T**( -2.000400E-01))*DT
      DYSY=DYS/(YS*YS)
      DX 1=DY 1/YS-Y 1*DYSY
      DX 2=DY 2/YS-Y 2*DYSY
      DSUMP 1=+DP 1S 2*X 2+P 1S 2*DX 2
```

```
      DSUMP 2=+DP 2S 1*X 1+P 2S 1*DX 1
      DB 1=(DSUMP 1-SUMP 1*DX 1/X 1)/X 1
      DB 2=(DSUMP 2-SUMP 2*DX 2/X 2)/X 2
      T 1=(DRL 1-RL 1*DB 1/B 1)/B 1
      T 2=(DRL 2-RL 2*DB 2/B 2)/B 2
      DRLM=+T 1+T 2
      DRHLM(IC)=DRH*RLM+RH*DRLM
C  SOLVE FOR UV.
      SUM 1=+X 2*VD 1 2
      SUM 2=+X 1*VD 1 2
      B 1=X 1*SUM 1*  5.0000E-05
      B 2=X 2*SUM 2*  5.0000E-05
      T 1=-RH*(1.0-U 1)
      T 2=-RH*(1.0-U 2)
      FAC 1=T 1/B 1
      FAC 2=T 2/B 2
      V 1=FAC 1*DX 1
      V 2=FAC 2*DX 2
      UV 1=U 1*V 1
      UV 2=U 2*V 2
      DV=-UV 1-UV 2
      UV 1=UV 1+DV*U 1
      UV 2=UV 2+DV*U 2
      RHUV(1ST+ 1)=RH*UV 1
      RHUV(1ST+ 2)=RH*UV 2
C  SPACE DER OF DENSITY TIMES UV.
      DDY 1=DDU 1/  2.00
      DDY 2=DDU 2/ 28.00
      DDYS=+DDY 1+DDY 2
      DYSYSQ=(DYS/YS)**2
      DDX 1=(DDY 1-2.0*DY 1*DYS/YS+2.0*Y 1*DYSYSQ-Y 1*DDYS/YS)/YS
      DDX 2=(DDY 2-2.0*DY 2*DYS/YS+2.0*Y 2*DYSYSQ-Y 2*DDYS/YS)/YS
      DSUM 1=+DX 2*VD 1 2+X 2*DVD 1 2
      DT 1=-DRH*(1.0-U 1)+RH*DU 1
      DT 2=-DRH*(1.0-U 2)+RH*DU 2
      DFAC 1=DT 1/B 1-T 1*DB 1/(B 1*B 1)
      DFAC 2=DT 2/B 2-T 2*DB 2/(B 2*B 2)
      DV 1=DFAC 1*DX 1+FAC 1*DDX 1
      DV 2=DFAC 2*DX 2+FAC 2*DDX 2
      DUV 1=DU 1*V 1+U 1*UV 1
      DUV 2=DU 2*V 2+U 2*UV 2
      DDV=-DUV 1-DUV 2
      DUV 1=DUV 1+DV*DU 1+DDV*U 1
      DUV 2=DUV 2+DV*DU 2+DDV*U 2
      DRHUV(1ST+ 1)=DRH*UV 1+RH*DUV 1
      DRHUV(1ST+ 2)=DRH*UV 2+RH*DUV 2
C  FIND THE TIME DERIVATIVES.
      SP=ASP+BSP*TIME
  100 CONTINUE
      IF(KPDE.EQ.NPDE)GO TO 150
      RY=     1.0000000000E-03*R(KPDE)
      DY=-     2.0000000000E+01*DRHUV(IST+KPDE)
      FVAL=SP*UPH(KPDE)+DY+RY
      RETURN
  150 CONTINUE
      DU 1=UPH( 1)
      DU 2=-DU 1
```

```
      TL=     4.0000000000E+05*                                       F         173
     * (DRHLM(IC)*UPH(NPDE)+RHLM(IC)*UPH2(NPDE))                      F         174
      TD=-     2.0000000000E+01*UPH(NPDE)*( +C(IST+ 1)*RHUV(IST+ 1) + F         175
     * C(IST+ 2)*RHUV(IST+ 2))                                        F         176
      TR=-     1.0000000000E-06*( +R( 1)*H(IST+ 1) +R( 2)*H(IST+ 2))  F         177
      FVAL=SP*UPH(NPDE)+(TL+TR+TD)/CM(IC)                             F         178
      RETURN                                                          F         179
      END                                                             F         180
```

```
      PROGRAM LOADF(INPUT,OUTPUT,TAPE5=INPUT,TAPE6=OUTPUT,
     * TAPE3,TAPE9,TAPE15)
C  LOADF CREATES THE SUBROUTINE F IN FLSC.
      DIMENSION II(72)
      DIMENSION III(44)
      DIMENSION LB(25),W(25),AU(7,25),AL(7,25)
      DIMENSION ALD(25),BLD(25),ABD(25,25),BHD(25,25)
      DIMENSION AV(25),BV(25)
      DIMENSION LBPR(25)
      WRITE(3,1000)
 1000 FORMAT(1HC,2X,63HFOR THE COMPLETE TRANSPORT CASE, WE DO NOT WANT T
     *HE U VALUES OR)
      WRITE(3,1005)
 1005 FORMAT(1HC,2X,62HTHEIR FIRST DERIVATIVES TO BE ZERO.  THIS CAN LEA
     *D TO DIVISION)
      WRITE(3,1010)
 1010 FORMAT(1HC,2X,8HBY ZERO.)
      WRITE(3,1012)
 1012 FORMAT(6X,14HDO 5 K=1,NPDEM)
      WRITE(3,1014)
 1014 FORMAT(6X,32HIF(ABS(U(K)).LT.SMALL)U(K)=SMALL)
      WRITE(3,1016)
 1016 FORMAT(1X,1H5,4X,36HIF(ABS(UPH(K)).LT.SMALL)UPH(K)=SMALL)
      READ(5,12)NLINE
 12   FORMAT(1014)
C  NLINE IS THE NUMBER OF COMMENT LINES TO BE READ AND PRINTED.
      DO 20 K=1,NLINE
      READ(5,22)II
      WRITE(3,22)II
 20   CONTINUE
 22   FORMAT(72A1)
 24   FORMAT(/1X,72A1/)
      READ(5,12)NSPC
      NM=NSPC-1
      LBM=1H-
      LBU=2HU(
      LBP=1H)
      WRITE(3,1020)((LBM,LBU,K,LBP),K=1,NM)
 1020 FORMAT(6X,6HYN=1.0,8(A1,A2,I2,A1),A1,2(/5X,1H*,1X,
     *  8(A2,I2,A1,A1))  )
      WRITE(3,1025)
 1025 FORMAT(6X,33HCALL RT(U,YN,R,NPDE,KPDE,IC,KSKR) )
      WRITE(3,18)NSPC
 18   FORMAT(6X,4HIST=,I2,7H*(IC-1) )
      DO 30 K=1,NSPC
      READ(5,32)LB(K),W(K)
      WRITE(6,34)K,LB(K),W(K)
      READ(15,36)(AU(L,K),L=1,5),(III(L),L=1,5)
      WRITE(6,36)(AU(L,K),L=1,5),(III(L),L=1,5)
      READ(15,36)(AU(L,K),L=6,7),(AL(L,K),L=1,3),(III(L),L=1,5)
      WRITE(6,36)(AU(L,K),L=6,7),(AL(L,K),L=1,3),(III(L),L=1,5)
      READ(15,37)(AL(L,K),L=4,7),(III(L),L=1,20)
      WRITE(6,37)(AL(L,K),L=4,7),(III(L),L=1,20)
 30   CONTINUE
 32   FORMAT(A5,7F7.0)
 34   FORMAT(/2X,14,4X,A5,4X,F8.2/)
 36   FORMAT(5E15.8,5A1)
```

```
37    FORMAT(4E15.8,20A1)
      READ(5,232)TPN,PHN,TMN
232   FORMAT(1P3E12.4)
      WRITE(3,27)
27    FORMAT(6X,22HIF(KSKT.GT.1)GO TO 100)
      WRITE(3,28)
28    FORMAT(6X,22HIF(KSKR.GT.1)GO TO 125  )
      READ(5,12)NLINE
      DO 40 K=1,NLINE
      READ(5,22)11
      WRITE(3,22)11
40    CONTINUE
C  *************************
C  ENTHALPIES AND HEAT CAPACITIES.
C  *************************
      WRITE(3,42)
42    FORMAT(6X,24HIF(T.GT.1000.)GO TO 2000)
      DO 50 K=1,NSPC
      WRITE(3,52)K,AL(1,K),AL(2,K)
      WRITE(3,54)(AL(L,K),L=3,5)
      WRITE(3,62)K,AL(6,K),AL(1,K)
      WRITE(3,64)AL(2,K),AL(3,K)
      WRITE(3,66)AL(4,K),AL(5,K)
50    CONTINUE
52    FORMAT(6X,1HC,12,9H=1.9872*(,1PE16.8,4H+T*(,1PE16.8)
54    FORMAT(5X,1H*,1X,3(4H+T*(,1PE16.8),5H)))))
      WRITE(3,56)
56    FORMAT(6X,10HGO TO 3000)
      WRITE(3,58)
58    FORMAT(4H2000,2X,8HCONTINUE)
      DO 60 K=1,NSPC
      WRITE(3,52)K,AU(1,K),AU(2,K)
      WRITE(3,54)(AU(L,K),L=3,5)
      WRITE(3,62)K,AU(6,K),AU(1,K)
      WRITE(3,64)AU(2,K),AU(3,K)
      WRITE(3,66)AU(4,K),AU(5,K)
60    CONTINUE
62    FORMAT(6X,1HH,12,9H=1.9872*(,1PE16.8,4H+T*(,1PE16.8)
64    FORMAT(5X,1H*,1X,4H+T*(,1PE16.8,4H/2.0,4H+T*(,1PE16.8,4H/3.0)
66    FORMAT(5X,1H*,1X,4H+T*(,1PE16.8,4H/4.0,4H+T*(,1PE16.8,
     * 4H/5.0,6H))))))
      WRITE(3,68)
68    FORMAT(4H3000,2X,8HCONTINUE)
      WRITE(3,134)
134   FORMAT(1HC,2X,39HSPECIFIC HEATS AND SPECIFIC ENTHALPIES.  )
      DO 140 K=1,NSPC
      WRITE(3,142)K,K,W(K)
      WRITE(3,144)K,K,W(K)
140   CONTINUE
142   FORMAT(6X,6HC(1ST+,12,3H)=C,12,1H/,F6.2)
144   FORMAT(6X,6HH(1ST+,12,3H)=H,12,1H/,F6.2)
      WRITE(3,146)
146   FORMAT(1X,3H125,2X,8HCONTINUE)
C  *************************
C  THERMAL CONDUCTIVITIES AND BINARY DIFFUSION COEFFICIENTS.
C  READ IN VISCOSITY, THERMAL CONDUCTIVITY, AND BINARY DIFFUSION
C  COEFFICIENTS FROM A FILE CREATED BY VALUES, CY=6.
```

```
C  *************************                                      MAIN  116
      READ(5,12)NLINE                                             MAIN  117
      DO 72 K=1,NLINE                                             MAIN  118
      READ(5,22)II                                                MAIN  119
      WRITE(6,22)II                                               MAIN  120
   72 WRITE(3,22)II                                               MAIN  121
   79 FORMAT(1HC,5X,1HV,I2,1H=,1PE14.6,5H*(T**,1PE14.6,1H) )      MAIN  122
      READ(5,12)NLINE                                             MAIN  123
      DO 70 K=1,NLINE                                             MAIN  124
      READ(5,22)II                                                MAIN  125
      WRITE(3,22)II                                               MAIN  126
      WRITE(6,22)II                                               MAIN  127
   70 CONTINUE                                                    MAIN  128
      DO 80 K=1,NSPC                                              MAIN  129
      READ(9,82)AV(K),BV(K),III                                   MAIN  130
      WRITE(6,84)K,LB(K),AV(K),BV(K),III                          MAIN  131
      READ(9,82)ALD(K),BLD(K),III                                 MAIN  132
      WRITE(6,84)K,LB(K),ALD(K),BLD(K),III                        MAIN  133
   80 CONTINUE                                                    MAIN  134
   82 FORMAT(1P2E14.6,44A1)                                       MAIN  135
   84 FORMAT(/2X,I4,4X,A4,4X,1P2E14.6,44A1/)                      MAIN  136
      DO 78 K=1,NSPC                                              MAIN  137
      WRITE(3,79)K,AV(K),BV(K)                                    MAIN  138
   78 CONTINUE                                                    MAIN  139
      DO 90 K=1,NSPC                                              MAIN  140
      WRITE(3,92)K,ALD(K),BLD(K)                                  MAIN  141
   90 CONTINUE                                                    MAIN  142
   92 FORMAT(6X,2HRL,I2,1H=,1PE14.6,5H*(T**,1PE14.6,1H))          MAIN  143
      READ(5,12)NLINE                                             MAIN  144
      DO 100 K=1,NLINE                                            MAIN  145
      READ(5,22)II                                                MAIN  146
      WRITE(3,22)II                                               MAIN  147
      WRITE(6,22)II                                               MAIN  148
  100 CONTINUE                                                    MAIN  149
      NM=NSPC-1                                                   MAIN  150
      DO 110 I=1,NSPC                                             MAIN  151
      DO 110 J=I,NSPC                                             MAIN  152
      READ(9,82)ABD(I,J),BBD(I,J),III                             MAIN  153
      WRITE(6,112)I,J,LB(I),LB(J),ABD(I,J),BBD(I,J),III           MAIN  154
  110 CONTINUE                                                    MAIN  155
  112 FORMAT(/2X,I4,4X,I4,4X,A4,4X,A4,4X,1P2E14.6,44A1/)          MAIN  156
      READ(5,114)PRESS                                            MAIN  157
  114 FORMAT(F6.0)                                                MAIN  158
      WRITE(3,116)PRESS                                           MAIN  159
  116 FORMAT(1HC,2X,7HPRESS =,F6.2)                               MAIN  160
      DO 120 I=1,NM                                               MAIN  161
      IP=1+I                                                      MAIN  162
      DO 120 J=IP,NSPC                                            MAIN  163
      ABD(I,J)=ABD(I,J)/PRESS                                     MAIN  164
      WRITE(3,122)I,J,ABD(I,J),BBD(I,J)                           MAIN  165
  120 CONTINUE                                                    MAIN  166
  122 FORMAT(1HC,5X,1HD,2I2,1H=,1PE16.8,5H*(T**,1PE16.8,1H) )      MAIN  167
C  *************************                                      MAIN  168
C  SPACE DERIVATIVES.                                             MAIN  169
C  *************************                                      MAIN  170
      LBPL=1H+                                                    MAIN  171
      WRITE(3,148)                                                MAIN  172
```

```
 148   FORMAT(1HC,2X,18HSPACE DERIVATIVES.)
       NS=NSPC+1
       WRITE(3,149)NS
 149   FORMAT(6X,4HYS=Y,I2)
       DO 150 K=1,NSPC
       WRITE(3,152)K,K
 150   CONTINUE
 152   FORMAT(6X,1HX,I2,2H=Y,I2,3H/YS)
       DO 160 K=1,NM
       WRITE(3,162)K,K
       WRITE(3,164)K,K
       WRITE(3,166)K,K
 160   CONTINUE
 162   FORMAT(6X,1HU,I2,3H=U(,I2,1H))
 164   FORMAT(6X,2HDU,I2,5H=UPH(,I2,1H))
 166   FORMAT(6X,3HDDU,I2,6H=UPH2(,I2,1H))
       LBU=1HU
       WRITE(3,172)NSPC,((LBM,LBU,K),K=1,NM)
 172   FORMAT(6X,1HU,I2,4H=1.0,8(A1,A1,I2),A1,2(/5X,1H*,1X,
      *  8(A1,I2,A1)) )
       LBDU=2HDU
       WRITE(3,174)NSPC,((LBM,LBDU,K),K=1,NM)
 174   FORMAT(6X,2HDU,I2,1H=,8(A1,A2,I2),A1,2(/5X,1H*,1X,
      *  8(A2,I2,A1)) )
       LBDDU=3HDDU
       WRITE(3,176)NSPC,((LBM,LBDDU,K),K=1,NM)
 176   FORMAT(6X,3HDDU,I2,1H=,8(A1,A3,I2),A1,2(/5X,1H*,1X,
      *  8(A3,I2,A1)) )
       DO 180 K=1,NSPC
       WRITE(3,182)K,K,W(K)
 180   CONTINUE
 182   FORMAT(6X,2HDY,I2,3H=DU,I2,1H/,F6.2)
       LBDY=2HDY
       WRITE(3,186)((LBPL,LBDY,K),K=1,NSPC)
 186   FORMAT(6X,4HDYS=,8(A1,A2,I2),A1,2(/5X,1H*,1X,8(A2,I2,A1)) )
       PSR=PRESS/82.05
       WRITE(3,234)TPN,PHN,TMN
       WRITE(6,234)TPN,PHN,TMN
 234   FORMAT(1HC,2X,5HTPN =,1PE12.4,6X,5HPHN =,1PE12.4,6X,
      * 5HTMN =,1PE12.4)
       WRITE(3,226)TPN
 226   FORMAT(6X,13HDT=UPH(NPDE)*,1PE12.4)
       WRITE(3,242)PSR
 242   FORMAT(6X,5HDRH=-,1PE18.10,21H*(DT/T+DYS/YS)/(T*YS))
       DO 800 K=1,NSPC
       A=ALD(K)*BLD(K)
       B=BLD(K)-1.0
       WRITE(3,803)K,A,B
 800   CONTINUE
 803   FORMAT(6X,3HDRL,I2,1H=,1PE16.8,6H*(T**(,1PE16.8,5H))*DT)
       DO 805 K=1,NSPC
       A=1.0/ALD(K)
       B=-BLD(K)
       WRITE(3,808)K,A,B
 805   CONTINUE
 808   FORMAT(6X,2HVL,I2,1H=,1PE16.8,6H*(T**(,1PE16.8,2H)) )
       DO 809 K=1,NSPC
```

```
      A=1.0/ALD(K)
      B=-BLD(K)
      A=A*B
      B=B-1.0
      WRITE(3,813)K,A,B
  809 CONTINUE
  813 FORMAT(6X,3HDVL,I2,1H=,1PE16.8,6H*(T**(,1PE16.8,5H))*DT)
      DO 815 I=1,NSPC
      DO 815 J=1,NSPC
      IF(I.EQ.J)GO TO 815
      A=1.0/ABD(I,J)
      B=-BBD(I,J)
      WRITE(3,818)I,J,A,B
  815 CONTINUE
  818 FORMAT(6X,2HVD,2I2,1H=,1PE16.8,6H*(T**(,1PE16.8,2H)) )
      DO 820 I=1,NSPC
      DO 820 J=1,NSPC
      IF(I.EQ.J)GO TO 820
      A=1.0/ABD(I,J)
      B=-BBD(I,J)
      A=A*B
      B=B-1.0
      WRITE(3,822)I,J,A,B
  820 CONTINUE
  822 FORMAT(6X,3HDVD,2I2,1H=,1PE16.8,6H*(T**(,1PE16.8,5H))*DT)
C  *************************
C  SPECIFIC HEAT OF THE MIXTURE.
C  *************************
      WRITE(3,124)
  124 FORMAT(1HC,2X,44HSPECIFIC HEAT OF THE MIXTURE.  NTIS FORMULA. )
      LBC=6HC(IST+
      LBU=3H)*U
      WRITE(3,132)((LBPL,LBC,K,LBU,K),K=1,NSPC)
  132 FORMAT(6X,7HCM(IC)=,4(A1,A6,I2,A3,I2),A1,
     * 4(/5X,1H*,1X,4(A6,I2,A3,I2,A1)) )
C  *************************
C  THERMAL CONDUCTIVITY OF THE MIXTURE.
C  *************************
      WRITE(3,272)
      WRITE(3,274)
  272 FORMAT(1HC,2X,36HTHERMAL CONDUCTIVITY OF THE MIXTURE.)
  274 FORMAT(1HC,2X,46HAVERAGE OF LINEAR AND RECIPROCAL MIXING RULES. )
      LBX=1HX
      LBPL=1H+
      LBRL=3H*RL
      LBMIX=5HRLSUM
      WRITE(3,260)LBMIX,((LBPL,LBX,K,LBRL,K),K=1,NSPC)
  260 FORMAT(6X,A5,1H=,6(2A1,I2,A3,I2),A1,2(/5X,1H*,1X,
     * 8(A1,I2,A3,I2,A1)) )
      LBSRL=3H*VL
      LBMIX=5HRLSIV
      WRITE(3,260)LBMIX,((LBPL,LBX,K,LBSRL,K),K=1,NSPC)
      WRITE(3,265)
  265 FORMAT(6X,15HRLSIV=1.0/RLSIV )
      WRITE(3,270)
  270 FORMAT(6X,21HRLM=0.5*(RLSUM+RLSIV) )
      WRITE(3,306)
```

```
  306   FORMAT(6X,15HRHLM(IC)=RH*RLM)                                     MAIN     287
  C  ************************                                             MAIN     288
  C  DERIVATIVE OF THE THERMAL CONDUCTIVITY OF THE MIXTURE.               MAIN     289
  C  ************************                                             MAIN     290
        WRITE(3,312)                                                      MAIN     291
  312   FORMAT(1HC,2X,40HSPACE DER OF DENSITY TIMES THERMAL COND.)        MAIN     292
        WRITE(3,745)                                                      MAIN     293
  745   FORMAT(6X,16HDYSY=DYS/(YS*YS)   )                                 MAIN     294
        DO 750 K=1,NSPC                                                   MAIN     295
        WRITE(3,752)K,K,K                                                 MAIN     296
  750   CONTINUE                                                          MAIN     297
  752   FORMAT(6X,2HDX,I2,3H=DY,I2,5H/YS-Y,I2,5H*DYSY   )                 MAIN     298
        LBDRL=4H*DRL                                                      MAIN     299
        LBDX=2HDX                                                         MAIN     300
        LBMIX=5HDLSUM                                                     MAIN     301
        WRITE(3,760)LBMIX,((LBPL,LBX,K,LBDRL,K,LBPL,LBDX,K,LBRL,K),       MAIN     302
       * K=1,NSPC)                                                        MAIN     303
  760   FORMAT(6X,A5,1H=,2(2A1,I2,A4,I2,A1,A2,I2,A3,I2),A1,               MAIN     304
       * 6(/5X,1H*,1X,3(A1,I2,A4,I2,A1,A2,I2,A3,I2,A1)) )                 MAIN     305
        LBPAR=1H)                                                         MAIN     306
        LBMIX=5HDLSIV                                                     MAIN     307
        LBDVL=4H*DVL                                                      MAIN     308
        WRITE(3,765)LBMIX,((LBPL,LBDX,K,LBSRL,K,LBPL,LBX,K,LBDVL,K),      MAIN     309
       * K=1,NSPC)                                                        MAIN     310
  765   FORMAT(6X,A5,1H=,2(A1,A2,I2,A3,I2,2A1,I2,A4,I2),A1,               MAIN     311
       * 6(/5X,1H*,1X,3(A2,I2,A3,I2,2A1,I2,A4,I2,A1)) )                   MAIN     312
        WRITE(3,770)                                                      MAIN     313
  770   FORMAT(6X,24HDLSIV=-RLSIV*RLSIV*DLSIV )                           MAIN     314
        WRITE(3,775)                                                      MAIN     315
  775   FORMAT(6X,22HDRLM=0.5*(DLSUM+DLSIV) )                             MAIN     316
        WRITE(3,778)                                                      MAIN     317
  778   FORMAT(6X,25HDRHLM(IC)=DRH*RLM+RH*DRLM)                           MAIN     318
  C  ************************                                             MAIN     319
  C  SOLVE FOR UV.                                                        MAIN     320
  C  HIRSHFELDER AND CURTISS APPROXIMATION.                               MAIN     321
  C  THE VELOCITY OF THE LAST SPECIES IS DETERMINED ONLY BY THE RELATION  MAIN     322
  C  SUM YI*VI = 0.0 .                                                    MAIN     323
  C  ************************                                             MAIN     324
        WRITE(3,400)                                                      MAIN     325
  400   FORMAT(1HC,2X,13HSOLVE FOR UV.)                                   MAIN     326
        LBX=1HX                                                           MAIN     327
        LBVD=3H*VD                                                        MAIN     328
        K=1                                                               MAIN     329
        WRITE(3,402)K,((LBPL,LBX,J,LBVD,K,J),J=2,NSPC)                    MAIN     330
  402   FORMAT(6X,3HSUM,I2,1H=,5(2A1,I2,A3,2I2),A1,                       MAIN     331
       * 3(/5X,1H*,1X,5(A1,I2,A3,2I2,A1)) )                               MAIN     332
        IF(NM.EQ.1)GO TO 412                                              LOADFX3    1
        DO 410 K=2,NM                                                     MAIN     333
        KM=K-1                                                            MAIN     334
        KP=K+1                                                            MAIN     335
        WRITE(3,402)K,((LBPL,LBX,J,LBVD,J,K),J=1,KM),((LBPL,LBX,J,        MAIN     336
       * LBVD,K,J),J=KP,NSPC)                                             MAIN     337
  410   CONTINUE                                                          MAIN     338
  412   CONTINUE                                                          LOADFX3    2
        DO 415 K=1,NM                                                     MAIN     339
        WRITE(3,418)K,K,K,PMN                                             MAIN     340
  415   CONTINUE                                                          MAIN     341
```

```
  418   FORMAT(6X,1HB,I2,2H=X,12,4H*SUM,I2,1H*,1PE12.4)                 MAIN      342
        DO 420 K=1,NM                                                   MAIN      343
        WRITE(3,422)K,K                                                 MAIN      344
  420   CONTINUE                                                        MAIN      345
  422   FORMAT(6X,1HT,I2,11H=-RH*(1.0-U,I2,1H) )                        MAIN      346
        DO 425 K=1,NM                                                   MAIN      347
        WRITE(3,428)K,K,K                                               MAIN      348
  425   CONTINUE                                                        MAIN      349
  428   FORMAT(6X,3HFAC,I2,2H=T,I2,2H/B,I2)                             MAIN      350
        DO 465 K=1,NM                                                   MAIN      351
        WRITE(3,468)K,K,K                                               MAIN      352
  465   CONTINUE                                                        MAIN      353
  468   FORMAT(6X,1HV,I2,4H=FAC,12,3H*DX,I2)                            MAIN      354
        DO 470 K=1,NM                                                   MAIN      355
        WRITE(3,472)K,K,K                                               MAIN      356
  470   CONTINUE                                                        MAIN      357
  472   FORMAT(6X,2HUV,I2,2H=U,I2,2H*V,12)                              MAIN      358
        LBUV=2HUV                                                       MAIN      359
        LBM=1H-                                                         MAIN      360
        WRITE(3,476)NSPC,((LBM,LBUV,K),K=1,NM)                          MAIN      361
  476   FORMAT(6X,2HUV,I2,1H=,10(A1,A2,12),A1,/5X,1H*,1X,10(A2,12,A1))  MAIN      362
        DO 485 K=1,NSPC                                                 MAIN      363
        WRITE(3,488)K,K                                                 MAIN      364
  485   CONTINUE                                                        MAIN      365
  488   FORMAT(6X,9HRHUV(IST+,I2,7H)=RH*UV,I2)                          MAIN      366
C   ************************                                            MAIN      367
C   SOLVE FOR THE SPACE DERIVATIVE OF UV.                               MAIN      368
C   ************************                                            MAIN      369
        WRITE(3,522)                                                    MAIN      370
  522   FORMAT(1HC,2X,30HSPACE DER OF DENSITY TIMES UV.)                MAIN      371
        DO 500 K=1,NSPC                                                 MAIN      372
        WRITE(3,502)K,K,W(K)                                            MAIN      373
  500   CONTINUE                                                        MAIN      374
  502   FORMAT(6X,3HDDY,I2,4H=DDU,I2,1H/,F6.2)                          MAIN      375
        LBDDY=3HDDY                                                     MAIN      376
        WRITE(3,506)((LBPL,LBDDY,K),K=1,NSPC)                           MAIN      377
  506   FORMAT(6X,5HDDYS=,8(A1,A3,I2),A1,2(/5X,1H*,1X,8(A3,I2,A1)) )    MAIN      378
        WRITE(3,510)                                                    MAIN      379
  510   FORMAT(6X,18HDYSYSQ=(DYS/YS)**2 )                               MAIN      380
        DO 515 K=1,NSPC                                                 MAIN      381
        WRITE(3,518)K,K,K,K,K                                           MAIN      382
  515   CONTINUE                                                        MAIN      383
  518   FORMAT(6X,3HDDX,I2,5H=(DDY,I2,7H-2.0*DY,I2,13H*DYS/YS+2.0*Y,    MAIN      384
       * I2,9H*DYSYSQ-Y,I2,12H*DDYS/YS)/YS  )                           MAIN      385
        LBDX=2HDX                                                       MAIN      386
        LBVD=3H*VD                                                      MAIN      387
        LBDVD=4H*DVD                                                    MAIN      388
        LBX=1HX                                                         MAIN      389
        K=1                                                             MAIN      390
        WRITE(3,532)K,((LBPL,LBDX,J,LBVD,K,J,LBPL,LBX,J,LBDVD,K,J),J=2, MAIN      391
       * NSPC)                                                          MAIN      392
  532   FORMAT(6X,4HDSUM,I2,1H=,2(A1,A2,I2,A3,2I2,2A1,12,A4,2I2),A1,    MAIN      393
       * 9(/5X,1H*,1X,2(A2,12,A3,2I2,2A1,I2,A4,2I2,A1)) )               MAIN      394
        IF(NM.EQ.1)GO TO 537                                            LOADFX3     3
        DO 535 K=2,NM                                                   MAIN      395
        KM=K-1                                                          MAIN      396
        KP=K+1                                                          MAIN      397
```

```
  418  FORMAT(6X,1HB,I2,2H=X,I2,4H*SUM,I2,1H*,1PE12.4)            MAIN     342
       DO 420 K=1,NM                                              MAIN     343
       WRITE(3,422)K,K                                            MAIN     344
  420  CONTINUE                                                   MAIN     345
  422  FORMAT(6X,1HT,I2,11H=-RH*(1.0-U,I2,1H) )                   MAIN     346
       DO 425 K=1,NM                                              MAIN     347
       WRITE(3,428)K,K,K                                          MAIN     348
  425  CONTINUE                                                   MAIN     349
  428  FORMAT(6X,3HFAC,I2,2H=T,I2,2H/B,I2)                        MAIN     350
       DO 465 K=1,NM                                              MAIN     351
       WRITE(3,468)K,K,K                                          MAIN     352
  465  CONTINUE                                                   MAIN     353
  468  FORMAT(6X,1HV,I2,4H=FAC,I2,3H*UX,I2)                       MAIN     354
       DO 470 K=1,NM                                              MAIN     355
       WRITE(3,472)K,K,K                                          MAIN     356
  470  CONTINUE                                                   MAIN     357
  472  FORMAT(6X,2HUV,I2,2H=U,I2,2H*V,I2)                         MAIN     358
       LBUV=2HUV                                                  MAIN     359
       LBM=1H-                                                    MAIN     360
       WRITE(3,476)NSPC,((LBM,LBUV,K),K=1,NM)                     MAIN     361
  476  FORMAT(6X,2HUV,I2,1H=,10(A1,A2,I2),A1,/5X,1H*,1X,10(A2,I2,A1))  MAIN 362
       DO 485 K=1,NSPC                                            MAIN     363
       WRITE(3,488)K,K                                            MAIN     364
  485  CONTINUE                                                   MAIN     365
  488  FORMAT(6X,9HRHUV(IST+,I2,7H)=RH*UV,I2)                     MAIN     366
C   ************************                                      MAIN     367
C   SOLVE FOR THE SPACE DERIVATIVE OF UV.                         MAIN     368
C   ************************                                      MAIN     369
       WRITE(3,522)                                               MAIN     370
  522  FORMAT(1HC,2X,30HSPACE DER OF DENSITY TIMES UV.)           MAIN     371
       DO 500 K=1,NSPC                                            MAIN     372
       WRITE(3,502)K,K,W(K)                                       MAIN     373
  500  CONTINUE                                                   MAIN     374
  502  FORMAT(6X,3HDDY,I2,4H=DDU,I2,1H/,F6.2)                     MAIN     375
       LBDDY=3HDDY                                                MAIN     376
       WRITE(3,506)((LBPL,LBDDY,K),K=1,NSPC)                      MAIN     377
  506  FORMAT(6X,5HDDYS=,8(A1,A3,I2),A1,2(/5X,1H*,1X,8(A3,I2,A1)) )  MAIN   378
       WRITE(3,510)                                               MAIN     379
  510  FORMAT(6X,18HDYSYSQ=(DYS/YS)**2 )                          MAIN     380
       DO 515 K=1,NSPC                                            MAIN     381
       WRITE(3,518)K,K,K,K,K                                      MAIN     382
  515  CONTINUE                                                   MAIN     383
  518  FORMAT(6X,3HDDX,I2,5H=(DDY,I2,7H-2.0*DY,I2,13H*DYS/YS+2.0*Y,  MAIN   384
     * I2,9H*DYSYSQ-Y,I2,12H*DDYS/YS)/YS  )                       MAIN     385
       LBDX=2HDX                                                  MAIN     386
       LBVD=3H*VD                                                 MAIN     387
       LBDVD=4H*DVD                                               MAIN     388
       LBX=1HX                                                    MAIN     389
       K=1                                                        MAIN     390
       WRITE(3,532)K,((LBPL,LBDX,J,LBVD,K,J,LBPL,LBX,J,LBDVD,K,J),J=2,  MAIN 391
     * NSPC)                                                      MAIN     392
  532  FORMAT(6X,4HDSUM,I2,1H=,2(A1,A2,I2,A3,2I2,2A1,I2,A4,2I2),A1,  MAIN   393
     * 9(/5X,1H*,1X,2(A2,I2,A3,2I2,2A1,I2,A4,2I2,A1)) )           MAIN     394
       IF(NM.EQ.1)GO TO 537                                       LOADFX3    3
       DO 535 K=2,NM                                              MAIN     395
       KM=K-1                                                     MAIN     396
       KP=K+1                                                     MAIN     397
```

```
          WRITE(3,532)K,((LBPL,LBDX,J,LBVU,J,K,LBPL,LBX,J,LBDVD,J,K),J=1,KM) MAIN      398
         * ,((LBPL,LBDX,J,LBVU,K,J,LBPL,LBX,J,LBDVD,K,J),J=KP,NSPC)            MAIN      399
  535     CONTINUE                                                             MAIN      400
  537     CONTINUE                                                             LOADFX3     4
          DO 540 K=1,NM                                                        MAIN      401
          WRITE(3,542)K,PHN,K,K,K,K                                            MAIN      402
  540     CONTINUE                                                             MAIN      403
  542     FORMAT(6X,2HDB,I2,1H=,1PE12.4,4H*(DX,I2,4H*SUM,I2,2H+X,I2,           MAIN      404
         * 5H*DSUM,I2,1H) )                                                    MAIN      405
          DO 545 K=1,NM                                                        MAIN      406
          WRITE(3,548)K,K,K                                                    MAIN      407
  545     CONTINUE                                                             MAIN      408
  548     FORMAT(6X,2HDT,I2,12H=-DRH*(1.0-U,I2,7H)+RH*DU,I2)                   MAIN      409
          DO 550 K=1,NM                                                        MAIN      410
          WRITE(3,552)(K,L=1,7)                                                MAIN      411
  550     CONTINUE                                                             MAIN      412
  552     FORMAT(6X,4HDFAC,I2,1H=,2HDT,I2,2H/B,I2,2H-T,I2,3H*DB,I2,            MAIN      413
         * 3H/(B,I2,2H*B,I2,1H) )                                              MAIN      414
          DO 590 K=1,NM                                                        MAIN      415
          WRITE(3,592)K,K,K,K,K                                                MAIN      416
  590     CONTINUE                                                             MAIN      417
  592     FORMAT(6X,2HDV,I2,5H=DFAC,I2,3H*DX,I2,4H+FAC,I2,4H*DDX,I2)           MAIN      418
          DO 595 K=1,NM                                                        MAIN      419
          WRITE(3,598)K,K,K,K,K                                                MAIN      420
  595     CONTINUE                                                             MAIN      421
  598     FORMAT(6X,3HDUV,I2,3H=DU,I2,2H*V,I2,2H+U,I2,3H*DV,I2)                MAIN      422
          LBDUV=3HDUV                                                          MAIN      423
          WRITE(3,802)NSPC,((LBM,LBDUV,K),K=1,NM)                              MAIN      424
  802     FORMAT(6X,3HDUV,I2,1H=,6(A1,A3,I2),A1,2(/5X,1H*,1X,                  MAIN      425
         * 9(A3,I2,A1)) )                                                      MAIN      426
          DO 810 K=1,NSPC                                                      MAIN      427
          WRITE(3,812)K,K,K                                                    MAIN      428
  810     CONTINUE                                                             MAIN      429
  812     FORMAT(6X,10HDRHUV(IST+,I2,8H)=DRH*UV,I2,7H+RH*DUV,I2)               MAIN      430
  C  ************************                                                  MAIN      431
  C  FIND THE TIME DERIVATIVES.                                                MAIN      432
  C  ************************                                                  MAIN      433
          WRITE(3,612)                                                         MAIN      434
  612     FORMAT(1HC,2X,26HFIND THE TIME DERIVATIVES.)                         MAIN      435
          WRITE(3,622)                                                         MAIN      436
  622     FORMAT(6X,15HSP=ASP+BSP*TIME)                                        MAIN      437
          TMSPH2=TMN/(PHN*PHN)                                                 MAIN      438
          WRITE(3,628)                                                         MAIN      439
  628     FORMAT(1X,3H100,2X,8HCONTINUE)                                       MAIN      440
          WRITE(3,632)                                                         MAIN      441
  632     FORMAT(6X,25HIF(KPDE.EQ.NPDE)GO TO 150)                              MAIN      442
          WRITE(3,636)TMN                                                      MAIN      443
  636     FORMAT(6X,3HRY=,1PE20.10,8H*R(KPDE) )                                MAIN      444
          TMSPH=TMN/PHN                                                        MAIN      445
          WRITE(3,638)TMSPH                                                    MAIN      446
  638     FORMAT(6X,4HDY=-,1PE20.10,16H*DRHUV(IST+KPDE) )                      MAIN      447
          WRITE(3,642)                                                         MAIN      448
  642     FORMAT(6X,23HFVAL=SP*UPH(KPDE)+DY+RY)                                MAIN      449
          WRITE(3,646)                                                         MAIN      450
  646     FORMAT(6X,6HRETURN)                                                  MAIN      451
          WRITE(3,648)                                                         MAIN      452
  648     FORMAT(1X,3H150,2X,8HCONTINUE)                                       MAIN      453
```

```
      DO 650 K=1,NM
      WRITE(3,652)K,K
  650 CONTINUE
  652 FORMAT(6X,2HDU,I2,5H=UPH(,I2,1H) )
      K=NSPC
      LBDU=2HDU
      WRITE(3,656)K,((LBM,LBDU,J),J=1,NM)
  656 FORMAT(6X,2HDU,I2,1H=,8(A1,A2,I2),AI,2(/5X,1H*,1X,8(A2,12,AI)) )
      WRITE(3,662)TMSPH2
  662 FORMAT(6X,3HTL=,IPE20.I0,1H*)
      WRITE(3,664)
  664 FORMAT(5X,IH*,1X,41H(DRHLM(IC)*UPH(NPDE)+RHLM(IC)*UPH2(NPDE)) )
      LBBL=IH
      LBC=6HC(IST+
      LBRHUV=10H)*RHUV(IST
      WRITE(3,668)TMSPH,((LBBL,LBPL,LBC,K,LBRHUV,LBPL,K,LBP),K=I,
     * NSPC),LBP
  668 FORMAT(6X,4HTD=-,1PE20.10,12H*UPH(NPDE)*(,2A1,A6,I2,AI0,A1,12,
     * 3AI,10(/5X,1H*,1X,2(A6,I2,A10,A1,12,3A1)) )
      TMSTP=TMN/TPN
      LBR=2HR(
      LBH=8H)*H(IST+
      WRITE(3,672)TMSTP,((LBBL,LBPL,LBR,K,LBH,K,LBP),K=I,NSPC),LBP
  672 FORMAT(6X,4HTR=-,IPE20.10,2H*(,2(2A1,A2,I2,A8,I2,AI),2A1,
     * 9(/5X,IH*,IX,2(A2,I2,A8,12,3AI)) )
      WRITE(3,676)
  676 FORMAT(6X,35HFVAL=SP*UPH(NPDE)+(TL+TR+TD)/CM(IC) )
      STOP
      END
```

```
     S C O P E   2   L O A D   M A P                              LOADER VERSION 1.0    04/15/80  14.10.30.  PAGE    1

PROGRAM  WILL BE ENTERED AT  LOADF      (   241)                  SCM LENGTH     15234          LCM LENGTH          0

         BLOCK         ADDRESS    LENGTH      FILE

         LOADF           110      10331       LGO
          /STP.END/     10441         1     SL-FTNLIB
          /FCL.C./      10442        30     SL-FTNLIB
          /Q8.IO./      10472       144     SL-FTNLIB
         Q2NTRY=        10636         4     SL-FTNLIB
         COMIO=         10642        10     SL-FTNLIB
         FECMSK=        10652        41     SL-FTNLIB
         FEIFST=        10713         3     SL-FTNLIB
         FLTIN=         10716       156     SL-FTNLIB
         FLTOUT=        11074       315     SL-FTNLIB
         FMTAP=         11411       377     SL-FTNLIB
         FORSYS=        12010       300     SL-FTNLIB
         FORUTL=        12310        45     SL-FTNLIB
         GETFIT=        12355        54     SL-FTNLIB
         INCOM=         12431       144     SL-FTNLIB
         INPC=          12575       173     SL-FTNLIB
         KODER=         12770       476     SL-FTNLIB
         KRAKER=        13466       454     SL-FTNLIB
         OUTC=          14142       155     SL-FTNLIB
         OUTCOM=        14317       204     SL-FTNLIB
         ERRCAP=        14523       317     SL-FTNLIB
         FERCAP=        15042       171     SL-FTNLIB
         SYSAID=        15233         1     SL-FTNLIB

    1    H2            2.00

 .31001901E+01  .51119464E-03  .52644210E-07 -.34909973E-10  .36945345E-14   H2
-.87738042E+03 -.19629421E+01  .30574451E+01  .26765200E-02 -.58099162E-05   H2
 .55210391E-08 -.18122739E-11 -.98890474E+03 -.22997056E+01                  H2

    2    N2           28.00

 .28963194E+01  .15154866E-02 -.57235277E-06  .99807393E-10 -.65223555E-14   N2
-.90586184E+03  .61615148E+01  .36748261E+01 -.12081500E-02  .23240102E-05   N2
-.63217559E-09 -.22577253E-12 -.10611588E+04  .23580424E+01                  N2
  VISCOSITY FROM WARNATZ ST PAR.
  LEAST SQUARES FIT,   T=300,2000.
  THERMAL CONDUCTIVITIES FROM WARNATZ ST PAR.
  LEAST SQUARES FIT,   T=300,2000.

    1    H2         2.188700E-06  6.502900E-01     H2       VISCOSITY.

    1    H2         6.357900E-06  7.383300E-01     H2       THERMAL CONDUCTIVITY.

    2    N2         4.266700E-06  6.613600E-01     N2       VISCOSITY.

    2    N2         6.407700E-07  7.999600E-01     N2       THERMAL CONDUCTIVITY.

  BINARY DIFFUSION COEFFICIENTS FROM WARNATZ ST PAR.
  LEAST SQUARES FIT.   T=300,2000.
```

```
1        2   H2    N2       5.951700E-05  1.663800E+00    H2        N2     BINARY DIFFUSION.

2        2   N2    N2       1.537400E-05  1.672900E+00    N2        N2     BINARY DIFFUSION.
TPN =  1.0000E+03      PHN =  5.0000E-05      TMN =  1.0000E-03
```

```
      SUBROUTINE F(TIME,PH,U,UPH,UPH2,FVAL,NPDE,KPDE,IC,KSKT,KSKR)          F
      DIMENSION U(NPDE),UPH(NPDE),UPH2(NPDE)                                F
      COMMON/TARAB/ASP,BSP,TPN,PHN,TMN,TMSPH,TMSPH2,TMSTP,TPENT             F
      COMMON/TARP/PRESS,PSR,NPDEM                                           F
      COMMON/TABSM/SMALL                                                    F
      DIMENSION R(20)                                                       F
      DIMENSION C(1000),H(1000),RHLM(100),DRHLM(100),CM(100)                F
      COMMON/TABCT/RL,CPMX,HO(20),R2D(20),R2DM(20)                          F
      COMMON/TABMF/RHUV(1000),DRHUV(1000)                                   F
      COMMON/TABRY/T,RH,Y1,Y2,Y3,Y4,Y5,Y6,Y7,Y8,Y9,Y10                      F
C  AT EACH CALL THE TIME RATE OF CHANGE FOR ONE PDE IS RETURNED IN FVAL.  F
C  FOR THE COMPLETE TRANSPORT CASE, WE DO NOT WANT THE U VALUES OR        F
C  THEIR FIRST DERIVATIVES TO BE ZERO.  THIS CAN LEAD TO DIVISION         F
C  BY ZERO.                                                               F
      DO 5 K=1,NPDEM                                                        F
      IF(ABS(U(K)).LT.SMALL)U(K)=SMALL                                      F
    5 IF(ABS(UPH(K)).LT.SMALL)UPH(K)=SMALL                                  F
C  TEST CASE.  BINARY MIX OF H2 AND N2.  TRANSPORT WARNATZ PAR.          F
C  U = MASS FRACTIONS.  Y = MASS FRACTIONS / MOLECULAR WEIGHTS.          F
      YN=1.0-U( 1)                                                          F
      CALL RT(U,YN,R,NPDE,KPDE,IC,KSKR)                                     F
      IST= 2*(IC-1)                                                         F
      IF(KSKT.GT.1)GO TO 100                                                F
      IF(KSKR.GT.1)GO TO 125                                                F
C  NTIS ENTHALPIES AND HEAT CAPACITIES.                                   F
      IF(T.GT.1000.)GO TO 2000                                              F
      C 1=1.9872*(  3.05744510E+00+T*(  2.67652000E-03                      F
     * +T*( -5.80991620E-06+T*(  5.52103910E-09+T*( -1.81227390E-12)))))  F
      H 1=1.9872*( -9.88904740E+02+T*(  3.05744510E+00                      F
     * +T*(  2.67652000E-03/2.0+T*( -5.80991620E-06/3.0                     F
     * +T*(  5.52103910E-09/4.0+T*( -1.81227390E-12/5.0))))))              F
      C 2=1.9872*(  3.67482610E+00+T*( -1.20815000E-03                      F
     * +T*(  2.32401020E-06+T*( -6.32175590E-10+T*( -2.25772530E-13)))))  F
      H 2=1.9872*( -1.06115880E+03+T*(  3.67482610E+00                      F
     * +T*( -1.20815000E-03/2.0+T*(  2.32401020E-06/3.0                     F
     * +T*( -6.32175590E-10/4.0+T*( -2.25772530E-13/5.0))))))              F
      GO TO 3000                                                            F
 2000 CONTINUE                                                              F
      C 1=1.9872*(  3.10019010E+00+T*(  5.11194640E-04                      F
     * +T*(  5.26442100E-08+T*( -3.49099730E-11+T*(  3.69453450E-15)))))  F
      H 1=1.9872*( -8.77380420E+02+T*(  3.10019010E+00                      F
     * +T*(  5.11194640E-04/2.0+T*(  5.26442100E-08/3.0                     F
     * +T*( -3.49099730E-11/4.0+T*(  3.69453450E-15/5.0))))))              F
      C 2=1.9872*(  2.89631940E+00+T*(  1.51548660E-03                      F
     * +T*( -5.72352770E-07+T*(  9.98073930E-11+T*( -6.52235550E-15)))))  F
      H 2=1.9872*( -9.05861840E+02+T*(  2.89631940E+00                      F
     * +T*(  1.51548660E-03/2.0+T*( -5.72352770E-07/3.0                     F
     * +T*(  9.98073930E-11/4.0+T*( -6.52235550E-15/5.0))))))              F
 3000 CONTINUE                                                              F
C  SPECIFIC HEATS AND SPECIFIC ENTHALPIES.                                F
      C(IST+ 1)=C 1/  2.00                                                  F
      H(IST+ 1)=H 1/  2.00                                                  F
      C(IST+ 2)=C 2/ 28.00                                                  F
      H(IST+ 2)=H 2/ 28.00                                                  F
  125 CONTINUE                                                              F
C  VISCOSITY FROM WARNATZ ST PAR.                                         F
C  LEAST SQUARES FIT,  T=300,2000.                                        F
```

```
C   THERMAL CONDUCTIVITIES FROM WARNATZ ST PAR.
C   LEAST SQUARES FIT,  T=300,2000.
C      V 1=  2.188700E-06*(T**  6.502900E-01)
C      V 2=  4.266700E-06*(T**  6.613600E-01)
       RL 1=  6.357900E-06*(T**  7.383300E-01)
       RL 2=  6.407700E-07*(T**  7.999600E-01)
C   BINARY DIFFUSION COEFFICIENTS FROM WARNATZ ST PAR.
C   LEAST SQUARES FIT,  T=300,2000.
C   PRESS =  1.00
C      D 1 2=  5.95170000E-05*(T**  1.66380000E+00)
C   SPACE DERIVATIVES.
       YS=Y 3
       X 1=Y 1/YS
       X 2=Y 2/YS
       U 1=U( 1)
       DU 1=UPH( 1)
       DDU 1=UPH2( 1)
       U 2=1.0-U 1
       DU 2=-DU 1
       DDU 2=-DDU 1
       DY 1=DU 1/  2.00
       DY 2=DU 2/ 28.00
       DYS=+DY 1+DY 2
C   TPN =  1.0000E+03       PHN =  5.0000E-05       TMN =  1.0000E-03
       DT=UPH(NPDE)*  1.0000E+03
       DRH=-  1.2187690433E-02*(DT/T+DYS/YS)/(T*YS)
       DRL 1=  4.69422831E-06*(T**( -2.61670000E-01))*DT
       DRL 2=  5.12590369E-07*(T**( -2.00040000E-01))*DT
       VL 1=  1.57284638E+05*(T**( -7.38330000E-01))
       VL 2=  1.56062238E+06*(T**( -7.99960000E-01))
       DVL 1= -1.16127967E+05*(T**( -1.73833000E+00))*DT
       DVL 2= -1.24843548E+06*(T**( -1.79996000E+00))*DT
       VD 1 2=  1.68019221E+04*(T**( -1.66380000E+00))
       DVD 1 2= -2.79550381E+04*(T**( -2.66380000E+00))*DT
C   SPECIFIC HEAT OF THE MIXTURE.  NTIS FORMULA.
       CM(IC)=+C(IST+ 1)*U 1+C(IST+ 2)*U 2
C   THERMAL CONDUCTIVITY OF THE MIXTURE.
C   AVERAGE OF LINEAR AND RECIPROCAL MIXING RULES.
       RLSUM=+X 1*RL 1+X 2*RL 2
       RLSIV=+X 1*VL 1+X 2*VL 2
       RLSIV=1.0/RLSIV
       RLM=0.5*(RLSUM+RLSIV)
       RHLM(IC)=RH*RLM
C   SPACE DER OF DENSITY TIMES THERMAL COND.
       DYSY=DYS/(YS*YS)
       DX 1=DY 1/YS-Y 1*DYSY
       DX 2=DY 2/YS-Y 2*DYSY
       DLSUM=+X 1*DRL 1+DX 1*RL 1+X 2*DRL 2+DX 2*RL 2
       DLSIV=+DX 1*VL 1+X 1*DVL 1+DX 2*VL 2+X 2*DVL 2
       DLSIV=-RLSIV*RLSIV*DLSIV
       DRLM=0.5*(DLSUM+DLSIV)
       DRHLM(IC)=DRH*RLM+RH*DRLM
C   SOLVE FOR UV.
       SUM 1=+X 2*VD 1 2
       B 1=X 1*SUM 1*  5.0000E-05
       T 1=-RH*(1.0-U 1)
       FAC 1=T 1/B 1
```

```
      V 1=FAC 1*DX 1
      UV 1=U 1*V 1
      UV 2=-UV 1
      RHUV(1ST+ 1)=RH*UV 1
      RHUV(1ST+ 2)=RH*UV 2
C  SPACE DER OF DENSITY TIMES UV.
      DDY 1=DDU 1/  2.00
      DDY 2=DDU 2/ 28.00
      DDYS=+DDY 1+DDY 2
      DYSYSQ=(DYS/YS)**2
      DDX 1=(DDY 1-2.0*DY 1*DYS/YS+2.0*Y 1*DYSYSQ-Y 1*DDYS/YS)/YS
      DDX 2=(DDY 2-2.0*DY 2*DYS/YS+2.0*Y 2*DYSYSQ-Y 2*DDYS/YS)/YS
      DSUM 1=+DX 2*VD 1 2+X 2*DVD 1 2
      DB 1=  5.0000E-05*(DX 1*SUM 1+X 1*DSUM 1)
      DT 1=-DRH*(1.0-U 1)+RH*DU 1
      DFAC 1=DT 1/B 1-T 1*DB 1/(B 1*B 1)
      DV 1=DFAC 1*DX 1+FAC 1*DDX 1
      DUV 1=DU 1*V 1+U 1*DV 1
      DUV 2=-DUV 1
      DRHUV(1ST+ 1)=DRH*UV 1+RH*DUV 1
      DRHUV(1ST+ 2)=DRH*UV 2+RH*DUV 2
C  FIND THE TIME DERIVATIVES.
      SP=ASP+BSP*TIME
  100 CONTINUE
      IF(KPDE.EQ.NPDE)GO TO 150
      RY=     1.0000000000E-03*R(KPDE)
      DY=-     2.0000000000E+01*DRHUV(1ST+KPDE)
      FVAL=SP*UPH(KPDE)+DY+RY
      RETURN
  150 CONTINUE
      DU 1=UPH( 1)
      DU 2=-DU 1
      TL=     4.0000000000E+05*
     * (DRHLM(IC)*UPH(NPDE)+RHLM(IC)*UPH2(NPDE))
      TD=-     2.0000000000E+01*UPH(NPDE)*( +C(1ST+ 1)*RHUV(1ST+ 1) +
     * C(1ST+ 2)*RHUV(1ST+ 2))
      TR=-     1.0000000000E-06*( +R( 1)*H(1ST+ 1) +R( 2)*H(1ST+ 2))
      FVAL=SP*UPH(NPDE)+(TL+TR+TD)/CM(IC)
      RETURN
      END
```

```
      PROGRAM LOADF(INPUT,OUTPUT,TAPE5=INPUT,TAPE6=OUTPUT,               MAIN        2
     * TAPE3,TAPE9,TAPE15)                                               MAIN        3
C  LOADF CREATES THE SUBROUTINE F IN FLSC.                               MAIN        4
      DIMENSION II(72)                                                   MAIN        5
      DIMENSION III(44)                                                  MAIN        6
      DIMENSION LB(25),W(25),AU(7,25),AL(7,25)                           MAIN        7
      DIMENSION LBTHD(25)                                                MAIN        8
      DIMENSION ESK(25)                                                  MAIN        9
      DIMENSION ALD(25),BLU(25),ABD(25,25),BBD(25,25)                    MAIN       10
      DIMENSION AV(25),BV(25)                                            MAIN       11
      DIMENSION LBPR(25)                                                 MAIN       12
      DIMENSION SGA(25),UM(25),ALP(25)                                   MAIN       13
C  BOLTZMAN CONSTANT.                                                    MAIN       14
      RK=1.38054E-16                                                     MAIN       15
      WRITE(3,1000)                                                      MAIN       16
1000  FORMAT(1HC,2X,63HFOR THE COMPLETE TRANSPORT CASE, WE DO NOT WANT T MAIN       17
     *HE U VALUES OR)                                                    MAIN       18
      WRITE(3,1005)                                                      MAIN       19
1005  FORMAT(1HC,2X,62HTHEIR FIRST DERIVATIVES TO BE ZERO.  THIS CAN LEA MAIN       20
     *D TO DIVISION)                                                     MAIN       21
      WRITE(3,1010)                                                      MAIN       22
1010  FORMAT(1HC,2X,8HBY ZERO.)                                          MAIN       23
      WRITE(3,1012)                                                      MAIN       24
1012  FORMAT(6X,14HDO 5 K=1,NPDEM)                                       MAIN       25
      WRITE(3,1014)                                                      MAIN       26
1014  FORMAT(6X,32HIF(ABS(U(K)).LT.SMALL)U(K)=SMALL)                     MAIN       27
      WRITE(3,1016)                                                      MAIN       28
1016  FORMAT(1X,1H5,4X,36HIF(ABS(UPH(K)).LT.SMALL)UPH(K)=SMALL)          MAIN       29
      READ(5,12)NLINE                                                    MAIN       30
12    FORMAT(10I4)                                                       MAIN       31
C  NLINE IS THE NUMBER OF COMMENT LINES TO BE READ AND PRINTED.          MAIN       32
      DO 20 K=1,NLINE                                                    MAIN       33
      READ(5,22)II                                                       MAIN       34
      WRITE(3,22)II                                                      MAIN       35
20    CONTINUE                                                           MAIN       36
22    FORMAT(72A1)                                                       MAIN       37
24    FORMAT(/1X,72A1/)                                                  MAIN       38
      READ(5,12)NSPC                                                     MAIN       39
      NM=NSPC-1                                                          MAIN       40
      LBM=1H-                                                            MAIN       41
      LBU=2HU(                                                           MAIN       42
      LBP=1H)                                                            MAIN       43
      WRITE(3,1020)((LBM,LBU,K,LBP),K=1,NM)                              MAIN       44
1020  FORMAT(6X,6HYN=1.0,8(A1,A2,I2,A1),A1,2(/5X,1H*,1X,                 MAIN       45
     *  8(A2,I2,A1,A1))   )                                              MAIN       46
      WRITE(3,1025)                                                      MAIN       47
1025  FORMAT(6X,33HCALL RT(U,YN,R,NPDE,KPDE,IC,KSKR) )                   MAIN       48
      WRITE(3,18)NSPC                                                    MAIN       49
18    FORMAT(6X,4HIST=,I2,7H*(IC-1) )                                    MAIN       50
      DO 30 K=1,NSPC                                                     MAIN       51
      READ(5,32)LB(K),LBTHD(K),W(K),SGA(K),ESK(K),UM(K),ALP(K)           MAIN       52
32    FORMAT(2A5,1P5E12.4)                                               MAIN       53
      WRITE(6,34)K,LB(K),LBTHD(K),W(K),SGA(K),ESK(K),UM(K),ALP(K)        MAIN       54
34    FORMAT(/5X,I4,2(5X,A5),1P5E12.4/)                                  MAIN       55
C  COMPUTE AN APPROXIMATION FOR THERMAL DIFFUSION FOR THOSE SPECIES      MAIN       56
C  WITH LBTHD = THDFF.                                                   MAIN       57
      READ(15,36)(AU(L,K),L=1,5),(III(L),L=1,5)                          MAIN       58
```

```
          WRITE(6,36)(AU(L,K),L=1,5),(III(L),L=1,5)
          READ(15,36)(AU(L,K),L=6,7),(AL(L,K),L=1,3),(III(L),L=I,5)
          WRITE(6,36)(AU(L,K),L=6,7),(AL(L,K),L=1,3),(III(L),L=1,5)
          READ(15,37)(AL(L,K),L=4,7),(III(L),L=1,20)
          WRITE(6,37)(AL(L,K),L=4,7),(III(L),L=I,20)
   30     CONTINUE
   36     FORMAT(5E15.8,5A1)
   37     FORMAT(4E15.8,20A1)
          READ(5,232)TPN,PHN,TMN
  232     FORMAT(IP3E12.4)
          WRITE(3,27)
   27     FORMAT(6X,22HIF(KSKT.GT.1)GO TO 100)
          WRITE(3,28)
   28     FORMAT(6X,22HIF(KSKR.GT.1)GO TO 125   )
          READ(5,I2)NLINE
          DO 40 K=I,NLINE
          READ(5,22)II
          WRITE(3,22)II
   40     CONTINUE
C    *************************
C    ENTHALPIES AND HEAT CAPACITIES.
C    *************************
          WRITE(3,42)
   42     FORMAT(6X,24HIF(T.GT.I000.)GO TO 2000)
          DO 50 K=1,NSPC
          WRITE(3,52)K,AL(1,K),AL(2,K)
          WRITE(3,54)(AL(L,K),L=3,5)
          WRITE(3,62)K,AL(6,K),AL(I,K)
          WRITE(3,64)AL(2,K),AL(3,K)
          WRITE(3,66)AL(4,K),AL(5,K)
   50     CONTINUE
   52     FORMAT(6X,1HC,I2,9H=1.9872*(,1PE16.8,4H+T*(,1PE16.8)
   54     FORMAT(5X,1H*,1X,3(4H+T*(,1PE16.8),5H))))))
          WRITE(3,56)
   56     FORMAT(6X,I0HGO TO 3000)
          WRITE(3,58)
   58     FORMAT(4H2000,2X,8HCONTINUE)
          DO 60 K=1,NSPC
          WRITE(3,52)K,AU(1,K),AU(2,K)
          WRITE(3,54)(AU(L,K),L=3,5)
          WRITE(3,62)K,AU(6,K),AU(1,K)
          WRITE(3,64)AU(2,K),AU(3,K)
          WRITE(3,66)AU(4,K),AU(5,K)
   60     CONTINUE
   62     FORMAT(6X,1HH,I2,9H=1.9872*(,IPE16.8,4H+T*(,1PE16.8)
   64     FORMAT(5X,1H*,1X,4H+T*(,1PE16.8,4H/2.0,4H+T*(,1PE16.8,4H/3.0)
   66     FORMAT(5X,1H*,1X,4H+T*(,1PE16.8,4H/4.0,4H+T*(,1PE16.8,
         * 4H/5.0,6H))))))
          WRITE(3,68)
   68     FORMAT(4H3000,2X,8HCONTINUE)
          WRITE(3,134)
  134     FORMAT(1HC,2X,39HSPECIFIC HEATS AND SPECIFIC ENTHALPIES.   )
          DO 140 K=1,NSPC
          WRITE(3,142)K,K,W(K)
          WRITE(3,144)K,K,W(K)
  140     CONTINUE
  142     FORMAT(6X,6HC(IST+,I2,3H)=C,I2,1H/,F6.2)
```

```
 144  FORMAT(6X,6HH(IST+,I2,3H)=H,I2,1H/,F6.2)
      WRITE(3,146)
 146  FORMAT(1X,3HI25,2X,8HCONTINUE)
C     ************************
C     THERMAL CONDUCTIVITIES AND BINARY DIFFUSION COEFFICIENTS.
C     READ IN VISCOSITY, THERMAL CONDUCTIVITY, AND BINARY DIFFUSION
C     COEFFICIENTS FROM A FILE CREATED BY VALUES, CY=6.
C     ************************
      READ(5,12)NLINE
      DO 72 K=1,NLINE
      READ(5,22)II
      WRITE(6,22)II
  72  WRITE(3,22)II
  79  FORMAT(1HC,5X,1HV,I2,1H=,1PE14.6,5H*(T**,1PE14.6,1H) )
      READ(5,12)NLINE
      DO 70 K=1,NLINE
      READ(5,22)II
      WRITE(3,22)II
      WRITE(6,22)II
  70  CONTINUE
      DO 80 K=1,NSPC
      READ(9,82)AV(K),BV(K),III
      WRITE(6,84)K,LB(K),AV(K),BV(K),III
      READ(9,82)ALD(K),BLD(K),III
      WRITE(6,84)K,LB(K),ALD(K),BLD(K),III
  80  CONTINUE
  82  FORMAT(1P2E14.6,44A1)
  84  FORMAT(/2X,I4,4X,A4,4X,1P2E14.6,44A1/)
      DO 78 K=1,NSPC
      WRITE(3,79)K,AV(K),BV(K)
  78  CONTINUE
      DO 90 K=1,NSPC
      WRITE(3,92)K,ALD(K),BLD(K)
  90  CONTINUE
  92  FORMAT(6X,2HRL,I2,1H=,1PE14.6,5H*(T**,1PE14.6,1H))
      READ(5,12)NLINE
      DO 100 K=1,NLINE
      READ(5,22)II
      WRITE(3,22)II
      WRITE(6,22)II
 100  CONTINUE
      NM=NSPC-1
      DO 110 I=1,NSPC
      DO 110 J=1,NSPC
      READ(9,82)ABD(I,J),BBD(I,J),III
      WRITE(6,112)I,J,LB(I),LB(J),ABD(I,J),BBD(I,J),III
 110  CONTINUE
 112  FORMAT(/2X,I4,4X,I4,4X,A4,4X,A4,4X,1P2E14.6,44A1/)
      READ(5,114)PRESS
 114  FORMAT(F6.0)
      WRITE(3,116)PRESS
 116  FORMAT(1HC,2X,7HPRESS =,F6.2)
      DO 120 I=1,NM
      IP=I+1
      DO 120 J=IP,NSPC
      ABD(I,J)=ABD(I,J)/PRESS
      WRITE(3,122)I,J,ABD(I,J),BBD(I,J)
```

```
  120   CONTINUE
  122   FORMAT(1HC,5X,1HD,2I2,1H=,1PE14.6,5H*(I**,1PE14.6,1H) )
        READ(5,279)ARTP,CRTP,III
        WRITE(6,123)ARTP,CRTP,III
        READ(5,279)ACST,CCST,III
        WRITE(6,123)ACST,CCST,III
  279   FORMAT(1P2E14.6,44A1)
  123   FORMAT(/2X,1P2E14.6,44A1)
C ************************
C SPACE DERIVATIVES.
C ************************
        LBPL=1H+
        WRITE(3,148)
  148   FORMAT(1HC,2X,18HSPACE DERIVATIVES.)
        NS=NSPC+1
        WRITE(3,149)NS
  149   FORMAT(6X,4HYS=Y,I2)
        DO 150 K=1,NSPC
        WRITE(3,152)K,K
  150   CONTINUE
  152   FORMAT(6X,1HX,I2,2H=Y,I2,3H/YS)
        DO 160 K=1,NM
        WRITE(3,162)K,K
        WRITE(3,164)K,K
        WRITE(3,166)K,K
  160   CONTINUE
  162   FORMAT(6X,1HU,I2,3H=U(,I2,1H))
  164   FORMAT(6X,2HDU,I2,5H=UPH(,I2,1H))
  166   FORMAT(6X,3HDDU,I2,6H=UPH2(,I2,1H))
        LBU=1HU
        WRITE(3,172)NSPC,((LBM,LBU,K),K=1,NM)
  172   FORMAT(6X,1HU,I2,4H=1.0,8(A1,A1,I2),A1,2(/5X,1H*,1X,
     *  8(A1,I2,A1)) )
        LBDU=2HDU
        WRITE(3,174)NSPC,((LBM,LBDU,K),K=1,NM)
  174   FORMAT(6X,2HDU,I2,1H=,8(A1,A2,I2),A1,2(/5X,1H*,1X,
     *  8(A2,I2,A1)) )
        LBDDU=3HDDU
        WRITE(3,176)NSPC,((LBM,LBDDU,K),K=1,NM)
  176   FORMAT(6X,3HDDU,I2,1H=,8(A1,A3,I2),A1,2(/5X,1H*,1X,
     *  8(A3,I2,A1)) )
        DO 180 K=1,NSPC
        WRITE(3,182)K,K,W(K)
  180   CONTINUE
  182   FORMAT(6X,2HDY,I2,3H=DU,I2,1H/,F6.2)
        LBDY=2HDY
        WRITE(3,186)((LBPL,LBDY,K),K=1,NSPC)
  186   FORMAT(6X,4HDYS=,8(A1,A2,I2),A1,2(/5X,1H*,1X,8(A2,I2,A1)) )
        PSR=PRESS/82.05
        WRITE(3,234)TPN,PHN,TMN
        WRITE(6,234)TPN,PHN,TMN
  234   FORMAT(1HC,2X,5HTPN =,1PE12.4,6X,5HPHN =,1PE12.4,6X,
     *  5HTMN =,1PE12.4)
        WRITE(3,226)TPN
  226   FORMAT(6X,13HDT=UPH(NPDE)*,1PE12.4)
        WRITE(3,227)TPN
  227   FORMAT(6X,15HDDT=UPH2(NPDE)*,1PE12.4)
```

```
      WRITE(3,242)PSR
  242 FORMAT(6X,5HDRH=-,1PE18.10,21H*(DT/T+DYS/YS)/(T*YS))
      DO 807 K=1,NSPC
      A=1.0/ALD(K)
      B=-BLD(K)
      WRITE(3,809)K,A,B
  807 CONTINUE
  809 FORMAT(6X,2HVL,12,1H=,1PE16.8,6H*(T**(,1PE16.8,2H)) )
      DO 740 K=1,NSPC
      A=ALD(K)*BLD(K)
      B=BLD(K)-1.0
      WRITE(3,742)K,A,B
  740 CONTINUE
  742 FORMAT(6X,3HDRL,12,1H=,1PE14.6,6H*(T**(,1PE14.6,5H))*DT  )
      DO 747 K=1,NSPC
      A=1.0/ALD(K)
      B=-BLD(K)
      A=A*B
      B=B-1.0
      WRITE(3,749)K,A,B
  747 CONTINUE
  749 FORMAT(6X,3HDVL,12,1H=,1PE14.6,6H*(T**(,1PE14.6,5H))*DT )
      WRITE(3,745)
  745 FORMAT(6X,16HDYSY=DYS/(YS*YS)  )
      DO 750 K=1,NSPC
      WRITE(3,752)K,K,K
  750 CONTINUE
  752 FORMAT(6X,2HDX,12,3H=DY,12,5H/YS-Y,I2,5H*DYSY  )
      DO 500 K=1,NSPC
      WRITE(3,502)K,K,W(K)
  500 CONTINUE
  502 FORMAT(6X,3HDDY,12,4H=DDU,12,1H/,F6.2)
      LBDDY=3HDDY
      WRITE(3,506)((LBPL,LBDDY,K),K=1,NSPC)
  506 FORMAT(6X,5HDDYS=,8(A1,A3,12),A1,2(/5X,1H*,1X,8(A3,I2,A1)) )
      WRITE(3,510)
  510 FORMAT(6X,18HDYSYSQ=(DYS/YS)**2 )
      DO 515 K=1,NSPC
      WRITE(3,518)K,K,K,K,K
  515 CONTINUE
  518 FORMAT(6X,3HDDX,12,5H=(DDY,12,7H-2.0*DY,I2,13H*DYS/YS+2.0*Y,
     * 12,9H*DYSYSQ-Y,12,12H*DDYS/YS)/YS  )
      DO 815 I=1,NSPC
      DO 815 J=I,NSPC
      IF(1.EQ.J)GO TO 815
      A=1.0/ABD(1,J)
      B=-BBD(1,J)
      WRITE(3,818)1,J,A,B
  815 CONTINUE
  818 FORMAT(6X,2HVD,2I2,1H=,1PE16.8,6H*(T**(,1PE16.8,2H)) )
      DO 820 I=1,NSPC
      DO 820 J=1,NSPC
      IF(I.EQ.J)GO TO 820
      A=1.0/ABD(I,J)
      B=-BBD(I,J)
      A=A*B
      B=B-1.0
```

```
      WRITE(3,822)I,J,A,B
  820 CONTINUE
  822 FORMAT(6X,3HDVD,2I2,1H=,1PE16.8,6H*(T**(,1PE16.8,5H))*DT)
C     ************************
C     SPECIFIC HEAT OF THE MIXTURE.
C     ************************
      WRITE(3,124)
  124 FORMAT(1HC,2X,44HSPECIFIC HEAT OF THE MIXTURE.  NTIS FORMULA. )
      LBC=6HC(IST+
      LBU=3H)*U
      WRITE(3,132)((LBPL,LBC,K,LBU,K),K=1,NSPC)
  132 FORMAT(6X,7HCM(IC)=,4(A1,A6,I2,A3,I2),A1,
     * 4(/5X,1H*,1X,4(A6,I2,A3,I2,A1)) )
C     ************************
C     THERMAL CONDUCTIVITY OF THE MIXTURE.
C     ************************
      WRITE(3,272)
      WRITE(3,274)
  272 FORMAT(1HC,2X,36HTHERMAL CONDUCTIVITY OF THE MIXTURE.)
  274 FORMAT(1HC,2X,46HAVERAGE OF LINAER AND RECIPROCAL MIXING RULES.  )
      LBX=1HX
      LBPL=1H+
      LBRL=3H*RL
      LBMIX=5HRLSUM
      WRITE(3,260)LBMIX,((LBPL,LBX,K,LBRL,K),K=1,NSPC)
  260 FORMAT(6X,A5,1H=,6(2A1,I2,A3,I2) ,A1,2(/5X,1H*,1X,
     * 8(A1,I2,A3,I2,A1)) )
      LBSRL=3H*VL
      LBMIX=5HRLSIV
      WRITE(3,260)LBMIX,((LBPL,LBX,K,LBSRL,K),K=1,NSPC)
      WRITE(3,265)
  265 FORMAT(6X,15HRLSIV=1.0/RLSIV  )
      WRITE(3,270)
  270 FORMAT(6X,21HRLM=0.5*(RLSUM+RLSIV))
      WRITE(3,306)
  306 FORMAT(6X,15HRHLM(IC)=RH*RLM  )
C     ************************
C     DERIVATIVE OF THE THERMAL CONDUCTIVITY OF THE MIXTURE.
C     ************************
      WRITE(3,312)
  312 FORMAT(1HC,2X,40HSPACE DER OF DENSITY TIMES THERMAL COND.)
      LBDRL=4H*DRL
      LBDX=2HDX
      LBMIX=5HDLSUM
      WRITE(3,760)LBMIX,((LBPL,LBX,K,LBDRL,K,LBPL,LBDX,K,LBRL,K),
     * K=1,NSPC)
  760 FORMAT(6X,A5,1H=,2(2A1,I2,A4,I2,A1,A2,I2,A3,I2),A1,6(/5X,1H*,1X,
     * 3(A1,I2,A4,I2,A1,A2,I2,A3,I2,A1)) )
      LBPAR=1H)
      LBMIX=5HDLSIV
      LBDVL=4H*DVL
      WRITE(3,765)LBMIX,((LBPL,LBDX,K,LBSRL,K,LBPL,LBX,K,LBDVL,K),
     * K=1,NSPC)
  765 FORMAT(6X,A5,1H=,2(A1,A2,I2,A3,I2,2A1,I2,A4,I2),A1,6(/5X,1H*,1X,
     * 3(A2,I2,A3,I2,2A1,I2,A4,I2,A1)) )
      WRITE(3,770)
  770 FORMAT(6X,24HDLSIV=-RLSIV*RLSIV*DLSIV  )
```

```
      WRITE(3,775)                                                   MAIN   344
  775 FORMAT(6X,22HDRLM=0.5*(DLSUM+DLSIV) )                          MAIN   345
      WRITE(3,778)                                                   MAIN   346
  778 FORMAT(6X,25HDRHLM(IC)=DRH*RLM+RH*DRLM )                       MAIN   347
C     ************************                                       MAIN   348
C     SOLVE FOR UV.                                                  MAIN   349
C     ZERO ORDER BORIS AND ORAN APPROXIMATION.                       MAIN   350
C     ************************                                       MAIN   351
      WRITE(3,400)                                                   MAIN   352
  400 FORMAT(IHC,2X,I3HSOLVE FOR UV.)                                MAIN   353
      LBX=IHX                                                        MAIN   354
      LBVD=3H*VD                                                     MAIN   355
      K=1                                                            MAIN   356
      WRITE(3,402)K,((LBPL,LBX,J,LBVD,K,J),J=2,NSPC)                 MAIN   357
  402 FORMAT(6X,3HSUM,I2,1H=,5(2A1,I2,A3,2I2),AI,3(/5X,IH*,IX,       MAIN   358
     * 5(A1,I2,A3,2I2,AI)) )                                         MAIN   359
      IF(NM.EQ.I)GO TO 412                                           TPC      1
      DO 410 K=2,NM                                                  MAIN   360
      KM=K-1                                                         MAIN   361
      KP=K+I                                                         MAIN   362
      WRITE(3,402)K,((LBPL,LBX,J,LBVD,J,K),J=1,KM),((LBPL,LBX,J,     MAIN   363
     * LBVD,K,J),J=KP,NSPC)                                          MAIN   364
  410 CONTINUE                                                       MAIN   365
  412 CONTINUE                                                       TPC      2
      K=NSPC                                                         MAIN   366
      WRITE(3,402)K,((LBPL,LBX,J,LBVD,J,K),J=I,NM)                   MAIN   367
      DO 415 K=I,NSPC                                                MAIN   368
      WRITE(3,418)K,K,K,PHN                                          MAIN   369
  415 CONTINUE                                                       MAIN   370
  418 FORMAT(6X,IHB,I2,2H=X,I2,4H*SUM,I2,IH*,1PE12.4)                MAIN   371
      DO 420 K=I,NSPC                                                MAIN   372
      WRITE(3,422)K,K                                                MAIN   373
  420 CONTINUE                                                       MAIN   374
  422 FORMAT(6X,IHT,I2,11H=-RH*(I.0-U,I2,1H) )                       MAIN   375
      DO 425 K=1,NSPC                                                MAIN   376
      WRITE(3,428)K,K,K                                              MAIN   377
  425 CONTINUE                                                       MAIN   378
  428 FORMAT(6X,3HFAC,I2,2H=T,I2,2H/B,I2)                            MAIN   379
      DO 465 K=1,NSPC                                                MAIN   380
      WRITE(3,468)K,K,K                                              MAIN   381
  465 CONTINUE                                                       MAIN   382
  468 FORMAT(6X,2HVX,I2,4H=FAC,I2,3H*DX,I2 )                         MAIN   383
      DO I200 K=I,NSPC                                               MAIN   384
      WRITE(3,I202)K,K,K                                             MAIN   385
 I200 CONTINUE                                                       MAIN   386
 1202 FORMAT(6X,3HUVX,I2,2H=U,I2,3H*VX,I2 )                          MAIN   387
C     ************************                                       MAIN   388
C     SOLVE FOR THE SPACE DERIVATIVE OF UV.                          MAIN   389
C     ************************                                       MAIN   390
      WRITE(3,522)                                                   MAIN   391
  522 FORMAT(IHC,2X,30HSPACE DER OF DENSITY TIMES UV.)               MAIN   392
      LBDX=2HDX                                                      MAIN   393
      LBVD=3H*VD                                                     MAIN   394
      LBX=IHX                                                        MAIN   395
      LBDVD=4H*DVD                                                   MAIN   396
      K=1                                                            MAIN   397
      WRITE(3,532)K,((LBPL,LBDX,J,LBVD,K,J,LBPL,LBX,J,LBDVD,K,J),    MAIN   398
```

```
          * J=2,NSPC)                                                   MAIN     399
  532     FORMAT(6X,4HDSUM,I2,1H=,2(A1,A2,I2,A3,2I2,2A1,I2,A4,2I2),A1,  MAIN     400
         * 9(/5X,1H*,1X,2(A2,I2,A3,2I2,2A1,I2,A4,2I2,A1)) )             MAIN     401
          IF(NM.EQ.1)GO TO 537                                          TPC        3
          DO 535 K=2,NM                                                 MAIN     402
          KM=K-1                                                        MAIN     403
          KP=K+1                                                        MAIN     404
          WRITE(3,532)K,((LBPL,LBDX,J,LBVD,J,K,LBPL,LBX,J,LBDVD,J,K),   MAIN     405
         * J=1,KM),((LBPL,LBDX,J,LBVD,K,J,LBPL,LBX,J,LBDVD,K,J),J=KP,NSPC) MAIN  406
  535     CONTINUE                                                      MAIN     407
  537     CONTINUE                                                      TPC        4
          K=NSPC                                                        MAIN     408
          WRITE(3,532)K,((LBPL,LBDX,J,LBVD,J,K,LBPL,LBX,J,LBDVD,J,K),J=1,NM) MAIN 409
          DO 540 K=1,NSPC                                               MAIN     410
          WRITE(3,542)K,PHN,K,K,K,K                                     MAIN     411
  540     CONTINUE                                                      MAIN     412
  542     FORMAT(6X,2HDB,I2,1H=,1PE12.4,4H*(DX,I2,4H*SUM,I2,2H+X,I2,    MAIN     413
         * 5H*DSUM,I2,1H) )                                             MAIN     414
          DO 545 K=1,NSPC                                               MAIN     415
          WRITE(3,548)K,K,K                                             MAIN     416
  545     CONTINUE                                                      MAIN     417
  548     FORMAT(6X,2HDT,I2,12H=-DRH*(1.0-U,I2,7H)+RH*DU,I2)            MAIN     418
          DO 550 K=1,NSPC                                               MAIN     419
          WRITE(3,552)(K,L=1,7)                                         MAIN     420
  550     CONTINUE                                                      MAIN     421
  552     FORMAT(6X,4HDFAC,I2,1H=,2HDT,I2,2H/B,I2,2H-T,I2,3H*DB,I2,     MAIN     422
         * 3H/(B,I2,2H*B,I2,1H) )                                       MAIN     423
          DO 590 K=1,NSPC                                               MAIN     424
          WRITE(3,592)K,K,K,K,K                                         MAIN     425
  590     CONTINUE                                                      MAIN     426
  592     FORMAT(6X,3HDVX,I2,5H=DFAC,I2,3H*DX,I2,4H+FAC,I2,4H*DDX,I2)   MAIN     427
          DO 595 K=1,NSPC                                               MAIN     428
  595     WRITE(3,598)K,K,K,K,K                                         MAIN     429
  598     FORMAT(6X,4HDUVX,I2,3H=DU,I2,3H*VX,I2,2H+U,I2,4H*DVX,I2)      MAIN     430
C   ************************                                            MAIN     431
C   USE A BINARY APPROXIMATION FOR THERMAL DIFFUSION FOR THE            MAIN     432
C   INDICATED SPECIES.                                                  MAIN     433
C   ************************                                            MAIN     434
C   WRITE THE NECESSARY ALPHA I J, WHERE I IS A SPECIES WE WANT TO      MAIN     435
C   COMPUTE THE THERMAL DIFFUSION FOR.                                  MAIN     436
C   ************************                                            MAIN     437
          WRITE(3,901)                                                  MAIN     438
  901     FORMAT(1HC,2X,40HCOMPUTE ALPHA FOR THE APPROPRIATE PAIRS. )   MAIN     439
          LBDFF=5HTHDFF                                                 MAIN     440
          DO 900 I=1,NM                                                 MAIN     441
          IPL=I+1                                                       MAIN     442
          DO 900 J=IPL,NSPC                                             MAIN     443
          IF(LBTHD(I).NE.LBDFF.AND.LBTHD(J).NE.LBDFF)GOTO900            MAIN     444
          IF(LBTHD(I).EQ.LBDFF)IP=I                                     MAIN     445
          IF(LBTHD(I).EQ.LBDFF)JP=J                                     MAIN     446
          IF(LBTHD(I).NE.LBDFF)IP=J                                     MAIN     447
          IF(LBTHD(I).NE.LBDFF)JP=I                                     MAIN     448
          E=SQRT(ESK(IP)*ESK(JP))                                       MAIN     449
          IF(UM(IP).EQ.0.0.AND.UM(JP).EQ.0.0)GO TO 1302                 MAIN     450
C   COMBINING RULE.  P. 528, REID AND SHERWOOD.                         MAIN     451
C   WE ARE ASSUMING AT MOST ONE POLAR SPECIES.                          MAIN     452
          IF(UM(IP).NE.0.0)LP=IP                                        MAIN     453
```

```
      IF(UM(JP).NE.0.0)LP=JP
      IF(LP.EQ.IP)LNP=JP
      IF(LP.EQ.JP)LNP=IP
      UMP=UM(LP)*1.0E-18
      SGC=SGA(LP)*1.0E-8
      TPSTAR=UMP*UMP/(ESK(LP)*RK*SGC*SGC*SGC*SQRT(8.0))
      FC=1.0+(1.0/SQRT(2.0))*(ALP(LNP)*TPSTAR/(SGA(LNP)**3))*SQRT(ESK(
     * LP)/ESK(LNP))
      WRITE(6,1305)IP,JP,LP,LNP,FC
 1305 FORMAT(/5X,4I6,1PE12.4)
      E=E*FC*FC
 1302 CONTINUE
      WRITE(3,903)E
  903 FORMAT(6X,5HTS=T/,1PE14.6)
      LBRTP=3HRTP
      WRITE(3,906)LBRTP,ARTP,CRTP
  906 FORMAT(6X,A3,1H=,1PE14.6,5H*EXP(,1PE14.6,4H/TS) )
      LBC=3HCST
      WRITE(3,906)LBC,ACST,CCST
      WRITE(3,909)
  909 FORMAT(6X,16HCSTP=6.0*CST-5.0 )
      WM=(W(IP)-W(JP))/(W(IP)+W(JP))
      WRITE(3,912)IP,JP,WM
  912 FORMAT(6X,2HAL,2I2,1H=,1PE14.6,9H*RTP*CSTP )
      WRITE(3,915)E
  915 FORMAT(6X,7HDTS=DT/,1PE14.6)
      A=-ARTP*CRTP
      LBDRTP=4HDRTP
      WRITE(3,918)LBDRTP,A,CRTP
  918 FORMAT(6X,A4,1H=,1PE14.6,5H*EXP(,1PE14.6,16H/TS)*DTS/(TS*TS) )
      LBDC=4HDCST
      A=-ACST*CCST
      WRITE(3,918)LBDC,A,CCST
      WRITE(3,921)
  921 FORMAT(6X,14HDCSTP=6.0*DCST )
      WRITE(3,924)IP,JP,WM
  924 FORMAT(6X,3HDAL,2I2,1H=,1PE14.6,22H*(DRTP*CSTP+RTP*DCSTP) )
      IF(LBTHD(JP).NE.LBDFF)GO TO 900
      WRITE(3,927)JP,IP,IP,JP
  927 FORMAT(6X,2HAL,2I2,2H=-,2HAL,2I2)
      WRITE(3,930)JP,IP,IP,JP
  930 FORMAT(6X,3HDAL,2I2,2H=-,3HDAL,2I2)
  900 CONTINUE
      WRITE(3,951)
  951 FORMAT(1HC,2X,48HCOMPUTE THERMAL DIFFUSION FOR THE GIVEN SPECIES.)
      LBX=1HX
      LBALP=3H*AL
      LBDX=2HDX
      LBDALP=4H*DAL
      DO 950 I=1,NSPC
      IF(LBTHD(I).NE.LBDFF)GO TO 950
      IF(I.EQ.1)WRITE(3,933)((LBPL,LBX,J,LBALP,I,J),J=2,NSPC)
  933 FORMAT(6X,4HSUM=,4(2A1,I2,A3,2I2),A1,4(/5X,1H*,IX,
     * 5(A1,I2,A3,2I2,A1)) )
      IF(I.EQ.NSPC)WRITE(3,933)((LBPL,LBX,J,LBALP,I,J),J=1,NM)
      IF(I.EQ.I.OR.I.EQ.NSPC)GO TO 93-
      IM=I-I
```

```
      IP=I+I
      WRITE(3,933)((LBPL,LBX,J,LBALP,I,J),J=1,IM),((LBPL,LBX,J,LBALP,
     * I,J),J=IP,NSPC)
 935  CONTINUE
      WRITE(3,936)I
 936  FORMAT(6X,5HRKT=X,I2,4H*SUM )
      WRITE(3,939)I
 939  FORMAT(6X,I2HVTOP=RKT*UVX,I2,3H*DT )
      WRITE(3,942)I
 942  FORMAT(6X,7HVBOT=DX,I2,2H*T )
      WRITE(3,945)I
 945  FORMAT(6X,3HUVT,I2,IOH=VTOP/VBOT )
      IF(I.EQ.I)WRITE(3,948)((LBPL,LBDX,J,LBALP,I,J,LBPL,LBX,J,LBDALP,I,
     * J),J=2,NSPC)
 948  FORMAT(6X,5HDSUM=,2(AI,A2,I2,A3,2I2,2AI,I2,A4,2I2),AI,
     * 8(/5X,IH*,IX,2(A2,I2,A3,2I2,2AI,I2,A4,2I2,AI)) )
      IF(I.EQ.NSPC)WRITE(3,948)((LBPL,LBDX,J,LBALP,I,J,LBPL,LBX,
     * J,LBDALP,I,J),J=I,NM)
      IF(I.EQ.I.OR.I.EQ.NSPC)GO TO 952
      IM=I-I
      IP=I+I
      WRITE(3,948)((LBPL,LBDX,J,LBALP,I,J,LBPL,LBX,J,LBDALP,I,J),
     * J=I,IM),((LBPL,LBDX,J,LBALP,I,J,LBPL,LBX,J,LBDALP,I,J),J=IP,NSPC)
 952  CONTINUE
      WRITE(3,955)I,I
 955  FORMAT(6X,7HDRKT=DX,I2,6H*SUM+X,I2,5H*DSUM )
      WRITE(3,958)I,I,I
 958  FORMAT(6X,I4HDVTOP=DRKT*UVX,I2,12H*DT+RKT*DUVX,I2,
     * I1H*DT+RKT*UVX,I2,4H*DDT )
      WRITE(3,96I)I,I
 96I  FORMAT(6X,9HDVBOT=DDX,I2,5H*T+DX,I2,3H*DT )
      WRITE(3,964)I
 964  FORMAT(6X,4HDUVT,I2,34H=DVTOP/VBOT-VTOP*DVBOT/(VBOT*VBOT) )
 950  CONTINUE
      WRITE(3,II29)
 II29 FORMAT(IHC,2X,36HFIND THE FINAL VALUES OF UV AND DUV.  )
      DO 1130 K=I,NSPC
      IF(LBTHD(K).EQ.LBDFF)WRITE(3,1132)K,K,K
      IF(LBTHD(K).NE.LBDFF)WRITE(3,II31)K,K
 II30 CONTINUE
 II31 FORMAT(6X,2HUV,I2,4H=UVX,I2)
 1I32 FORMAT(6X,2HUV,I2,4H=UVX,I2,4H+UVT,I2)
      DO II35 K=I,NSPC
      IF(LBTHD(K).EQ.LBOFF)WRITE(3,II38)K,K,K
      IF(LBTHD(K).NE.LBOFF)WRITE(3,1137)K,K
 II35 CONTINUE
 II37 FORMAT(6X,3HDUV,I2,5H=DUVX,I2)
 II38 FORMAT(6X,3HDUV,I2,5H=DUVX,I2,5H+DUVT,I2)
 995  CONTINUE
      LBUV=2HUV
      WRITE(3,1212)((LBM,LBUV,K),K=1,NSPC)
 1212 FORMAT(6X,3HDV=,8(AI,A2,I2),AI,2(/5X,1H*,1X,8(A2,I2,AI)) )
      DO 1215 K=1,NSPC
 1215 WRITE(3,1218)K,K,K
 1218 FORMAT(6X,2HUV,I2,3H=UV,I2,5H+DV*D,I2)
      LBDUV=3HDUV
      WRITE(3,1222)((LBM,LBDUV,K),K=1,NSPC)
```

```
      IP=I+1
      WRITE(3,933)((LBPL,LBX,J,LBALP,I,J),J=1,IM),((LBPL,LBX,J,LBALP,
     * I,J),J=IP,NSPC)
  935 CONTINUE
      WRITE(3,936)I
  936 FORMAT(6X,5HRKT=X,I2,4H*SUM )
      WRITE(3,939)I
  939 FORMAT(6X,12HVTOP=RKT*UVX,I2,3H*DT )
      WRITE(3,942)I
  942 FORMAT(6X,7HVBOT=DX,I2,2H*T )
      WRITE(3,945)I
  945 FORMAT(6X,3HUVT,I2,10H=VTOP/VBOT )
      IF(I.EQ.1)WRITE(3,948)((LBPL,LBDX,J,LBALP,I,J,LBPL,LBX,J,LBDALP,I,
     * J),J=2,NSPC)
  948 FORMAT(6X,5HDSUM=,2(A1,A2,I2,A3,2I2,2A1,I2,A4,2I2),A1,
     * 8(/5X,1H*,1X,2(A2,I2,A3,2I2,2A1,I2,A4,2I2,A1)) )
      IF(I.EQ.NSPC)WRITE(3,948)((LBPL,LBDX,J,LBALP,I,J,LBPL,LBX,
     * J,LBDALP,I,J),J=1,NM)
      IF(I.EQ.1.OR.I.EQ.NSPC)GO TO 952
      IM=I-1
      IP=I+1
      WRITE(3,948)((LBPL,LBDX,J,LBALP,I,J,LBPL,LBX,J,LBDALP,I,J),
     * J=1,IM),((LBPL,LBDX,J,LBALP,I,J,LBPL,LBX,J,LBDALP,I,J),J=IP,NSPC)
  952 CONTINUE
      WRITE(3,955)I,I
  955 FORMAT(6X,7HDRKT=DX,I2,6H*SUM+X,I2,5H*DSUM )
      WRITE(3,958)I,I,I
  958 FORMAT(6X,14HDVTOP=DRKT*UVX,I2,12H*DT+RKT*DUVX,I2,
     * 11H*DT+RKT*UVX,I2,4H*DDT )
      WRITE(3,961)I,I
  961 FORMAT(6X,9HDVBOT=DDX,I2,5H*T+DX,I2,3H*DT )
      WRITE(3,964)I
  964 FORMAT(6X,4HDUVT,I2,34H=DVTOP/VBOT-VTOP*DVBOT/(VBOT*VBOT) )
  950 CONTINUE
      WRITE(3,1129)
 1129 FORMAT(1HC,2X,36HFIND THE FINAL VALUES OF UV AND DUV.  )
      DO 1130 K=1,NSPC
      IF(LBTHD(K).EQ.LBDFF)WRITE(3,1132)K,K,K
      IF(LBTHD(K).NE.LBDFF)WRITE(3,1131)K,K
 1130 CONTINUE
 1131 FORMAT(6X,2HUV,I2,4H=UVX,I2)
 1132 FORMAT(6X,2HUV,I2,4H=UVX,I2,4H*UVT,I2)
      DO 1135 K=1,NSPC
      IF(LBTHD(K).EQ.LBDFF)WRITE(3,1138)K,K,K
      IF(LBTHD(K).NE.LBDFF)WRITE(3,1137)K,K
 1135 CONTINUE
 1137 FORMAT(6X,3HDUV,I2,5H=DUVX,I2)
 1138 FORMAT(6X,3HDUV,I2,5H=DUVX,I2,5H*DUVT,I2)
  995 CONTINUE
      LBUV=2HUV
      WRITE(3,1212)((LBM,LBUV,K),K=1,NSPC)
 1212 FORMAT(6X,3HDV=,8(A1,A2,I2),A1,2(/5X,1H*,1X,8(A2,I2,A1)) )
      DO 1215 K=1,NSPC
 1215 WRITE(3,1218)K,K,K
 1218 FORMAT(6X,2HUV,I2,3H=UV,I2,5H*DV*U,I2)
      LBDUV=3HDUV
      WRITE(3,1222)((LBM,LBDUV,K),K=1,NSPC)
```

```
 1222 FORMAT(6X,4HDDV=,8(A1,A3,I2),A1,2(/5X,1H*,1X,8(A3,I2,A1)) )
      DO 1225 K=1,NSPC
 1225 WRITE(3,1228)K,K,K,K
 1228 FORMAT(6X,3HDUV,I2,4H=DUV,I2,6H+DV*DU,I2,6H+DDV*U,I2)
      DO 485 K=1,NSPC
 485  WRITE(3,488)K,K
 488  FORMAT(6X,9HRHUV(IST+,I2,7H)=RH*UV,I2)
      DO 810 K=1,NSPC
 810  WRITE(3,812)K,K,K
 812  FORMAT(6X,10HDRHUV(IST+,I2,8H)=DRH*UV,I2,7H+RH*DUV,I2)
C     ************************
C     FIND THE TIME DERIVATIVES.
C     ************************
      WRITE(3,612)
 612  FORMAT(1HC,2X,26HFIND THE TIME DERIVATIVES.)
      WRITE(3,622)
 622  FORMAT(6X,15HSP=ASP+BSP*TIME)
      TMSPH2=TMN/(PHN*PHN)
      WRITE(3,628)
 628  FORMAT(1X,3H100,2X,8HCONTINUE)
      WRITE(3,632)
 632  FORMAT(6X,25HIF(KPDE.EQ.NPDE)GO TO 150)
      WRITE(3,636)TMN
 636  FORMAT(6X,3HRY=,1PE20.10,8H*R(KPDE) )
      TMSPH=TMN/PHN
      WRITE(3,638)TMSPH
 638  FORMAT(6X,4HDY=-,1PE20.10,16H*DRHUV(IST+KPDE) )
      WRITE(3,642)
 642  FORMAT(6X,23HFVAL=SP*UPH(KPDE)+DY+RY)
      WRITE(3,646)
 646  FORMAT(6X,6HRETURN)
      WRITE(3,648)
 648  FORMAT(1X,3H150,2X,8HCONTINUE)
      DO 650 K=1,NM
      WRITE(3,652)K,K
 650  CONTINUE
 652  FORMAT(6X,2HDU,I2,5H=UPH(,I2,1H) )
      K=NSPC
      LBDU=2HDU
      WRITE(3,656)K,((LBM,LBDU,J),J=1,NM)
 656  FORMAT(6X,2HDU,I2,1H=,8(A1,A2,I2),A1,2(/5X,1H*,1X,8(A2,I2,A1)) )
      WRITE(3,662)TMSPH2
 662  FORMAT(6X,3HTL=,1PE20.10,1H*)
      WRITE(3,664)
 664  FORMAT(5X,1H*,1X,41H(DRHLM(IC)*UPH(NPDE)+RHLM(IC)*UPH2(NPDE)) )
      LBBL=1H
      LBC=6HC(IST+
      LBRHUV=10H)*RHUV(IST
      WRITE(3,668)TMSPH,((LBBL,LBPL,LBC,K,LBRHUV,LBPL,K,LBP),K=1,
     * NSPC),LBP
 668  FORMAT(6X,4HTD=-,1PE20.10,12H*UPH(NPDE)*(,2A1,A6,I2,A10,A1,I2,
     * 3A1,10(/5X,1H*,1X,2(A6,I2,A10,A1,I2,3A1)) )
      TMSTP=TMN/TPN
      LBR=2HR(
      LBH=8H)*H(IST+
      WRITE(3,672)TMSTP,((LBBL,LBPL,LBR,K,LBH,K,LBP),K=1,NSPC),LBP
 672  FORMAT(6X,4HTR=-,1PE20.10,2H*(,2(2A1,A2,I2,A8,I2,A1),2A1,
```

```
      * 9(/5X,IH*,1X,2(A2,I2,A8,I2,3A1)) )                          MAIN   625
        WRITE(3,676)                                                MAIN   626
  676   FORMAT(6X,35HFVAL=SP*UPH(NPDE)+(IL+TR+TD)/CM(IC) )          MAIN   627
        STOP                                                        MAIN   628
        END                                                         MAIN   629
```

```
       S C O P E   2   L O A D   M A P                                   LOADER VERSION 1.0    04/15/80  13.55.48.  PAGE   1

PROGRAM  WILL BE ENTERED AT  LOADF      (    241)                        SCM LENGTH     17276          LCM LENGTH          0

       BLOCK          ADDRESS    LENGTH      FILE

       LOADF            110      12230        LGO
        /STP.END/     12340          1      SL-FTNLIB
        /FCL.C./      12341         30      SL-FTNLIB
        /Q8.IO./      12371        144      SL-FTNLIB
       Q2NTRY=        12535          4      SL-FTNLIB
       COMIO=         12541         10      SL-FTNLIB
       FECMSK=        12551         41      SL-FTNLIB
       FEIFST=        12612          3      SL-FTNLIB
       FLTIN=         12615        156      SL-FTNLIB
       FLTOUT=        12773        315      SL-FTNLIB
       FMTAP=         13310        377      SL-FTNLIB
       FORSYS=        13707        300      SL-FTNLIB
       FORUTL=        14207         45      SL-FTNLIB
       GETFIT=        14254         54      SL-FTNLIB
       INCOM=         14330        144      SL-FTNLIB
       INPC=          14474        173      SL-FTNLIB
       KODER=         14667        476      SL-FTNLIB
       KRAKER=        15365        454      SL-FTNLIB
       OUTC=          16041        155      SL-FTNLIB
       OUTCOM=        16216        204      SL-FTNLIB
       ERRCAP=        16422        317      SL-FTNLIB
       FERCAP=        16741        171      SL-FTNLIB
       EXP.MSG        17132         16      SL-FTNLIB
       SQRT           17150          6      SL-FTNLIB
       SQRT.          17156         32      SL-FTNLIB
       SYSAID=        17210          1      SL-FTNLIB
       SYS=1ST        17211         65      SL-FTNLIB

    1     H2          THDFF  2.0000E+00  2.9200E+00  3.8000E+01  0.          7.9000E-01

 .31001901E+01  .51119464E-03  .52644210E-07 -.34909973E-10  .36945345E-14    H2
-.87738042E+03 -.19629421E+01  .30574451E+01  .26765200E-02 -.58099162E-05    H2
 .55210391E-08 -.18122739E-11 -.98890474E+03 -.22997056E+01                   H2

    2     N2                 2.8000E+01  3.6200E+00  9.7500E+01  0.          0.

 .28963194E+01  .15154866E-02 -.57235277E-06  .99807393E-10 -.65223555E-14    N2
-.90586184E+03  .61615148E+01  .36748261E+01 -.12081500E-02  .23240102E-05    N2
-.63217559E-09 -.22577253E-12 -.10611588E+04  .23580424E+01                   N2
  VISCOSITY FROM WARNATZ ST PAR.
  LEAST SQUARES FIT,  T=300,2000.
  THERMAL CONDUCTIVITIES FROM WARNATZ ST PAR.
  LEAST SQUARES FIT,  T=300,2000.

   1    H2       2.188700E-06  6.502900E-01    H2     VISCOSITY.

   1    H2       6.357900E-06  7.383300E-01    H2     THERMAL CONDUCTIVITY.

   2    N2       4.266700E-06  6.613600E-01    N2     VISCOSITY.

   2    N2       6.407700E-07  7.999600E-01    N2     THERMAL CONDUCTIVITY.
```

```
BINARY DIFFUSION COEFFICIENTS FROM WARNATZ ST PAR.
LEAST SQUARES FIT.  T=100.300

 1      1    H2     H2        1.119300E-04  1.661400E+00   H2       H2     BINARY DIFFUSION.

 1      2    H2     N2        5.951700E-05  1.663800E+00   H2       N2     BINARY DIFFUSION.

 2      2    N2     N2        1.537400E-05  1.672900E+00   N2       N2     BINARY DIFFUSION.

 8.112200E-01  4.866900E-02   RTP=RT/(6C*-5)   FIT A*EXP(C/T)

 9.542600E-01 -1.435700E-01   C*  HCB  FIT  A*EXP(C/T)
TPN =  1.0000E+03      PHN =  5.0000E-05      TMN =  1.0000E-03
```

```
      SUBROUTINE F(TIME,PH,U,UPH,UPH2,FVAL,NPDE,KPDE,IC,KSKT,KSKR)
      DIMENSION U(NPDE),UPH(NPDE),UPH2(NPDE)
      COMMON/TARAB/ASP,BSP,TPN,PHN,TMN,TMSPH,TMSPH2,TMSTP,TPENT
      COMMON/TARP/PRESS,PSR,NPDEM
      COMMON/TARSM/SMALL
      DIMENSION R(20)
      DIMENSION C(1000),H(1000),RHLM(100),DRHLM(100),CM(100)
      COMMON/TABCT/RL,CPMX,HO(20),R2D(20),R2DM(20)
      COMMON/TARMF/RHUV(1000),DRHUV(1000)
      COMMON/TABRY/T,RH,Y1,Y2,Y3,Y4,Y5,Y6,Y7,Y8,Y9,Y10
C  AT EACH CALL THE TIME RATE OF CHANGE FOR ONE PDE IS RETURNED IN FVAL.
C  FOR THE COMPLETE TRANSPORT CASE, WE DO NOT WANT THE U VALUES OR
C  THEIR FIRST DERIVATIVES TO BE ZERO.  THIS CAN LEAD TO DIVISION
C  BY ZERO.
      DO 5 K=1,NPDEM
      IF(ABS(U(K)).LT.SMALL)U(K)=SMALL
    5 IF(ABS(UPH(K)).LT.SMALL)UPH(K)=SMALL
C  TEST CASE.  BINARY MIX OF H2 AND N2.  WARNATZ TRANSPORT VALUES.
      YN=1.0-U( 1)
      CALL RT(U,YN,R,NPDE,KPDE,IC,KSKR)
      IST= 2*(IC-1)
      IF(KSKT.GT.1)GO TO 100
      IF(KSKR.GT.1)GO TO 125
C  NTIS ENTHALPIES AND HEAT CAPACITIES.
      IF(T.GT.1000.)GO TO 2000
      C 1=1.9872*(  3.05744510E+00+T*(  2.67652000E-03
     * +T*( -5.80991620E-06+T*(  5.52103910E-09+T*( -1.81227390E-12)))))
      H 1=1.9872*( -9.88904740E+02+T*(  3.05744510E+00
     * +T*(  2.67652000E-03/2.0+T*( -5.80991620E-06/3.0
     * +T*(  5.52103910E-09/4.0+T*( -1.81227390E-12/5.0))))))
      C 2=1.9872*(  3.67482610E+00+T*( -1.20815000E-03
     * +T*(  2.32401020E-06+T*( -6.32175590E-10+T*( -2.25772530E-13)))))
      H 2=1.9872*( -1.06115880E+03+T*(  3.67482610E+00
     * +T*( -1.20815000E-03/2.0+T*(  2.32401020E-06/3.0
     * +T*( -6.32175590E-10/4.0+T*( -2.25772530E-13/5.0))))))
      GO TO 3000
 2000 CONTINUE
      C 1=1.9872*(  3.10019010E+00+T*(  5.11194640E-04
     * +T*(  5.26442100E-08+T*( -3.49099730E-11+T*(  3.69453450E-15)))))
      H 1=1.9872*( -8.77380420E+02+T*(  3.10019010E+00
     * +T*(  5.11194640E-04/2.0+T*(  5.26442100E-08/3.0
     * +T*( -3.49099730E-11/4.0+T*(  3.69453450E-15/5.0))))))
      C 2=1.9872*(  2.89631940E+00+T*(  1.51548660E-03
     * +T*( -5.72352770E-07+T*(  9.98073930E-11+T*( -6.52235550E-15)))))
      H 2=1.9872*( -9.05861840E+02+T*(  2.89631940E+00
     * +T*(  1.51548660E-03/2.0+T*( -5.72352770E-07/3.0
     * +T*(  9.98073930E-11/4.0+T*( -6.52235550E-15/5.0))))))
 3000 CONTINUE
C  SPECIFIC HEATS AND SPECIFIC ENTHALPIES.
      C(IST+ 1)=C 1/  2.00
      H(IST+ 1)=H 1/  2.00
      C(IST+ 2)=C 2/ 28.00
      H(IST+ 2)=H 2/ 28.00
  125 CONTINUE
C  VISCOSITY FROM WARNATZ ST PAR.
C  LEAST SQUARES FIT,  T=300,2000.
C  THERMAL CONDUCTIVITIES FROM WARNATZ ST PAR.
```

```
C  LEAST SQUARES FIT,  T=300,2000.
C     V 1=  2.188700E-06*(T**  6.502900E-01)
C     V 2=  4.266700E-06*(T**  6.613600E-01)
      RL 1=  6.357900E-06*(T**  7.383300E-01)
      RL 2=  6.407700E-07*(T**  7.999600E-01)
C  BINARY DIFFUSION COEFFICIENTS FROM WARNATZ ST PAR.
C  LEAST SQUARES FIT,  T=100,300
C  PRESS =  1.00
C     D 1 2=  5.951700E-05*(T**  1.663800E+00)
C  SPACE DERIVATIVES.
      YS=Y 3
      X 1=Y 1/YS
      X 2=Y 2/YS
      U 1=U( 1)
      DU 1=UPH( 1)
      DDU 1=UPH2( 1)
      U 2=1.0-U 1
      DU 2=-DU 1
      DDU 2=-DDU 1
      DY 1=DU 1/  2.00
      DY 2=DU 2/ 28.00
      DYS=+DY 1+DY 2
C  TPN =  1.0000E+03      PHN =  5.0000E-05      TMN =  1.0000E-03
      DT=UPH(NPDE)*  1.0000E+03
      DDT=UPH2(NPDE)*  1.0000E+03
      DRH=-  1.21876904 33E-02*(DT/T+DYS/YS)/(T*YS)
      VL 1=  1.57284638E+05*(T**( -7.38330000E-01))
      VL 2=  1.56062238E+06*(T**( -7.99960000E-01))
      DRL 1=  4.694228E-06*(T**( -2.616700E-01))*DT
      DRL 2=  5.125904E-07*(T**( -2.000400E-01))*DT
      DVL 1= -1.161280E+05*(T**( -1.738330E+00))*DT
      DVL 2= -1.248435E+06*(T**( -1.799960E+00))*DT
      DYSY=DYS/(YS*YS)
      DX 1=DY 1/YS-Y 1*DYSY
      DX 2=DY 2/YS-Y 2*DYSY
      DDY 1=DDU 1/  2.00
      DDY 2=DDU 2/ 28.00
      DDYS=+DDY 1+DDY 2
      DYSYSQ=(DYS/YS)**2
      DDX 1=(DDY 1-2.0*DY 1*DYS/YS+2.0*Y 1*DYSYSQ-Y 1*DDYS/YS)/YS
      DDX 2=(DDY 2-2.0*DY 2*DYS/YS+2.0*Y 2*DYSYSQ-Y 2*DDYS/YS)/YS
      VD 1 2=  1.68019221E+04*(T**( -1.66380000E+00))
      DVD 1 2= -2.79550381E+04*(T**( -2.66380000E+00))*DT
C  SPECIFIC HEAT OF THE MIXTURE.  NTIS FORMULA.
      CM(IC)=+C(IST+ 1)*U 1+C(IST+ 2)*U 2
C  THERMAL CONDUCTIVITY OF THE MIXTURE.
C  AVERAGE OF LINAER AND RECIPROCAL MIXING RULES.
      RLSUM=+X 1*RL 1+X 2*RL 2
      RLSIV=+X 1*VL 1+X 2*VL 2
      RLSIV=1.0/RLSIV
      RLM=0.5*(PLSUM+RLSIV)
      RHLM(IC)=RH*RLM
C  SPACE DER OF DENSITY TIMES THERMAL COND.
      DLSUM=+X 1*DRL 1+DX 1*RL 1+X 2*DRL 2+DX 2*RL 2
      DLSIV=+DX 1*VL 1+X 1*DVL 1+DX 2*VL 2+X 2*DVL 2
      DLSIV=-RLSIV*RLSIV*DLSIV
      DRLM=0.5*(DLSUM+DLSIV)
```

```
      DRHLM(IC)=DRH*RLM+RH*DRLM
C  SOLVE FOR UV.
      SUM 1=+X 2*VD 1 2
      SUM 2=+X 1*VD 1 2
      B 1=X 1*SUM 1*  5.0000E-05
      B 2=X 2*SUM 2*  5.0000E-05
      T 1=-RH*(1.0-U 1)
      T 2=-RH*(1.0-U 2)
      FAC 1=T 1/B 1
      FAC 2=T 2/B 2
      VX 1=FAC 1*DX 1
      VX 2=FAC 2*DX 2
      UVX 1=U 1*VX 1
      UVX 2=U 2*VX 2
C  SPACE DER OF DENSITY TIMES UV.
      DSUM 1=+DX 2*VD 1 2+X 2*DVD 1 2
      DSUM 2=+DX 1*VD 1 2+X 1*DVD 1 2
      DB 1=  5.0000E-05*(DX 1*SUM 1+X 1*DSUM 1)
      DB 2=  5.0000E-05*(DX 2*SUM 2+X 2*DSUM 2)
      DT 1=-DRH*(1.0-U 1)+RH*DU 1
      DT 2=-DRH*(1.0-U 2)+RH*DU 2
      DFAC 1=DT 1/B 1-T 1*DB 1/(B 1*B 1)
      DFAC 2=DT 2/B 2-T 2*DB 2/(B 2*B 2)
      DVX 1=DFAC 1*DX 1+FAC 1*DDX 1
      DVX 2=DFAC 2*DX 2+FAC 2*DDX 2
      DUVX 1=DU 1*VX 1+U 1*DVX 1
      DUVX 2=DU 2*VX 2+U 2*DVX 2
C  COMPUTE ALPHA FOR THE APPROPRIATE PAIRS.
      TS=T/  6.086871E+01
      RTP=  8.112200E-01*EXP(  4.866900E-02/TS)
      CST=  9.542600E-01*EXP( -1.435700E-01/TS)
      CSTP=6.0*CST-5.0
      AL 1 2= -8.666667E-01*RTP*CSTP
      DTS=DT/  6.086871E+01
      DRTP= -3.948127E-02*EXP(  4.866900E-02/TS)*DTS/(TS*TS)
      DCST=  1.370031E-01*EXP( -1.435700E-01/TS)*DTS/(TS*TS)
      DCSTP=6.0*DCST
      DAL 1 2= -8.666667E-01*(DRTP*CSTP+RTP*DCSTP)
C  COMPUTE THERMAL DIFFUSION FOR THE GIVEN SPECIES.
      SUM=+X 2*AL 1 2
      RKT=X 1*SUM
      VTOP=RKT*UVX 1*DT
      VBOT=DX 1*T
      UVT 1=VTOP/VBOT
      DSUM=+DX 2*AL 1 2+X 2*DAL 1 2
      DRKT=DX 1*SUM+X 1*DSUM
      DVTOP=DRKT*UVX 1*DT+RKT*DUVX 1*DT+RKT*UVX 1*DDT
      DVBOT=DDX 1*T+DX 1*DT
      DUVT 1=DVTOP/VBOT-VTOP*DVBOT/(VBOT*VBOT)
C  FIND THE FINAL VALUES OF UV AND DUV.
      UV 1=UVX 1+UVT 1
      UV 2=UVX 2
      DUV 1=DUVX 1+DUVT 1
      DUV 2=DUVX 2
      DV=-UV 1-UV 2
      UV 1=UV 1+DV*U 1
      UV 2=UV 2+DV*U 2
```

```
      DDV=-DUV 1-DUV 2
      DUV 1=DUV 1+DV*DU 1+DDV*U 1
      DUV 2=DUV 2+DV*DU 2+DDV*U 2
      RHUV(IST+ 1)=RH*UV 1
      RHUV(IST+ 2)=RH*UV 2
      DRHUV(IST+ 1)=DRH*UV 1+RH*DUV 1
      DRHUV(IST+ 2)=DRH*UV 2+RH*DUV 2
C  FIND THE TIME DERIVATIVES.
      SP=ASP+BSP*TIME
  100 CONTINUE
      IF(KPDE.EQ.NPDE)GO TO 150
      RY=    1.0000000000E-03*R(KPDE)
      DY=-    2.0000000000E+01*DRHUV(IST+KPDE)
      FVAL=SP*UPH(KPDE)+DY+RY
      RETURN
  150 CONTINUE
      DU 1=UPH( 1)
      DU 2=-DU 1
      TL=    4.0000000000E+05*
     * (DRHLM(IC)*UPH(NPDE)+RHLM(IC)*UPH2(NPDE))
      TD=-    2.0000000000E+01*UPH(NPDE)*( +C(IST+ 1)*RHUV(IST+ 1) +
     * C(IST+ 2)*RHUV(IST+ 2))
      TR=-    1.0000000000E-06*( +R( 1)*H(IST+ 1) +R( 2)*H(IST+ 2))
      FVAL=SP*UPH(NPDE)+(TL+TR+TD)/CM(IC)
      RETURN
      END
```

LIST OF SYMBOLS

$A^*_{ij} = \Omega^{(2,2)*}_{ij}/\Omega^{(1,1)*}_{ij}$, quotient of collision integrals.

$B^*_{ij} = [5\Omega^{(1,2)*}_{ij} - 4\Omega^{(1,3)*}_{ij}]/\Omega^{(1,1)*}_{ij}$, quotient of collision integrals.

$C^*_{ij} = \Omega^{(1,2)*}_{ij}/\Omega^{(1,1)*}_{ij}$, quotient of collison integrals.

$C_{i,int}$ = internal heat capacity, cal-mole^{-1}-K^{-1}.

$C_{i,rot}$ = rotational heat capacity, cal-mole^{-1}-K^{-1}.

$C_{i,tr}$ = translational heat capacity, cal-mole^{-1}-K^{-1}.

$C_{i,v}$ = heat capacity at constant volume, cal-mole^{-1}-K^{-1}.

c_{pi} = specific heat, cal-gm^{-1}-K^{-1}.

$c_p = \sum_{i=1}^{N} c_{pi}Y_i$, specific heat of the mixture, cal-gm^{-1}-K^{-1}.

$\mathcal{D}_{ij}$ = binary diffusion coefficient, cm^2-s^{-1}.

D_{im} = diffusion coefficient of species i into a mixture, cm^2-s^{-1}.

D_{ij} = multicomponent diffusion coefficient, cm^2-s^{-1}.

D_i^T = multicomponent thermal diffusion coefficient, gm-s^{-1}-cm^{-1}.

$\mathcal{D}_{i,int,j}$ = binary diffusion coefficient for internal energy, cm^2-s^{-1}.

h_i = specific enthalpy, cal-gm^{-1}.

k = Boltzmann constant = 1.38054X10^{-16} erg-K^{-1}-molecule^{-1}.

k_{ij} = thermal diffusion ratio.

k_{im} = thermal diffusion ratio between species i and the rest of the mixture.

M_i = molecular weight, gm-mole^{-1}.

p = pressure, atm.

q = total energy flux relative to the fluid velocity, cal-cm^{-2}-s^{-1}.

R_i = rate of production of ith species by chemical reaction, mole-cm^{-3}-s^{-1}.

R = gas constant = 1.9872 cal-mole^{-1}-K^{-1}.

R_a = gas constant = 82.05 cm^3-atm-mole^{-1}-K^{-1}.

t = time, s.

T = temperature, K.

T_u = temperature of unburned mixture, K.

T_B = temperature of burned mixture, K.

T_i^* = $T/(\varepsilon_i/k)$.

T_{ij}^* = $T/(\varepsilon_{ij}/k)$.

u = fluid velocity, cm-s^{-1}.

V_i = diffusion velocity, cm-s^{-1}.

$\mathcal{V}_i$ = diffusion velocity due to species gradients, cm-s^{-1}.

$\mathcal{W}_i$ = diffusion velocity due to the temperature gradient, cm-s^{-1}.

x = spatial coordinate, cm.

X_i = mole fraction.

Y_i = mass fraction.

Y_{iu} = mass fraction of species i in the unburned mixture.

Y_{iB} = mass fraction of species i in the burned mixture.

α_i = polarizibility, Å^3.

ε_i/k = Lennard-Jones or Stockmayer parameter, K.

η_i = viscosity, poise = gm-cm^{-1}-s^{-1}.

μ_i = dipole moment, debye = 10^{-18} gm$^{1/2}$-cm$^{5/2}$-s^{-1}.

σ_i = Lennard-Jones or Stockmayer parameter, Å.

λ_o = thermal conductivity of the mixtures, neglecting diffusion effects, cal-cm^{-1}-s^{-1}-K^{-1}.

$\lambda_{o,tr}$ = thermal conductivity due to translational energy, cal-cm^{-1}-s^{-1}-K^{-1}.

$\lambda_{o,int}$ = thermal conductivity due to internal energy, cal-cm^{-1}-s^{-1}-K^{-1}.

λ_{mix}^{mon} = thermal conductivity of a mixture of monatomic gases, cal-cm^{-1}-s^{-1}-K^{-1}.

λ_{mix}^{poly} = thermal conductivity of a mixture, cal-cm^{-1}-s^{-1}-K^{-1}.

ρ = fluid density, gm-cm^{-3}.

ξ_{ij} = rotational collision numbers.

$\Omega_{ij}^{(1,1)*}$; $\Omega_{ij}^{(2,2)*}$; $\Omega_{ij}^{(1,2)*}$; $\Omega_{ij}^{(1,3)*}$ = collision integral.

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